U.S. DEPARTMENT OF ENERGY | Office of Science

Overview of the Energy Frontier Research Centers Program

Dr. Altaf H. Carim

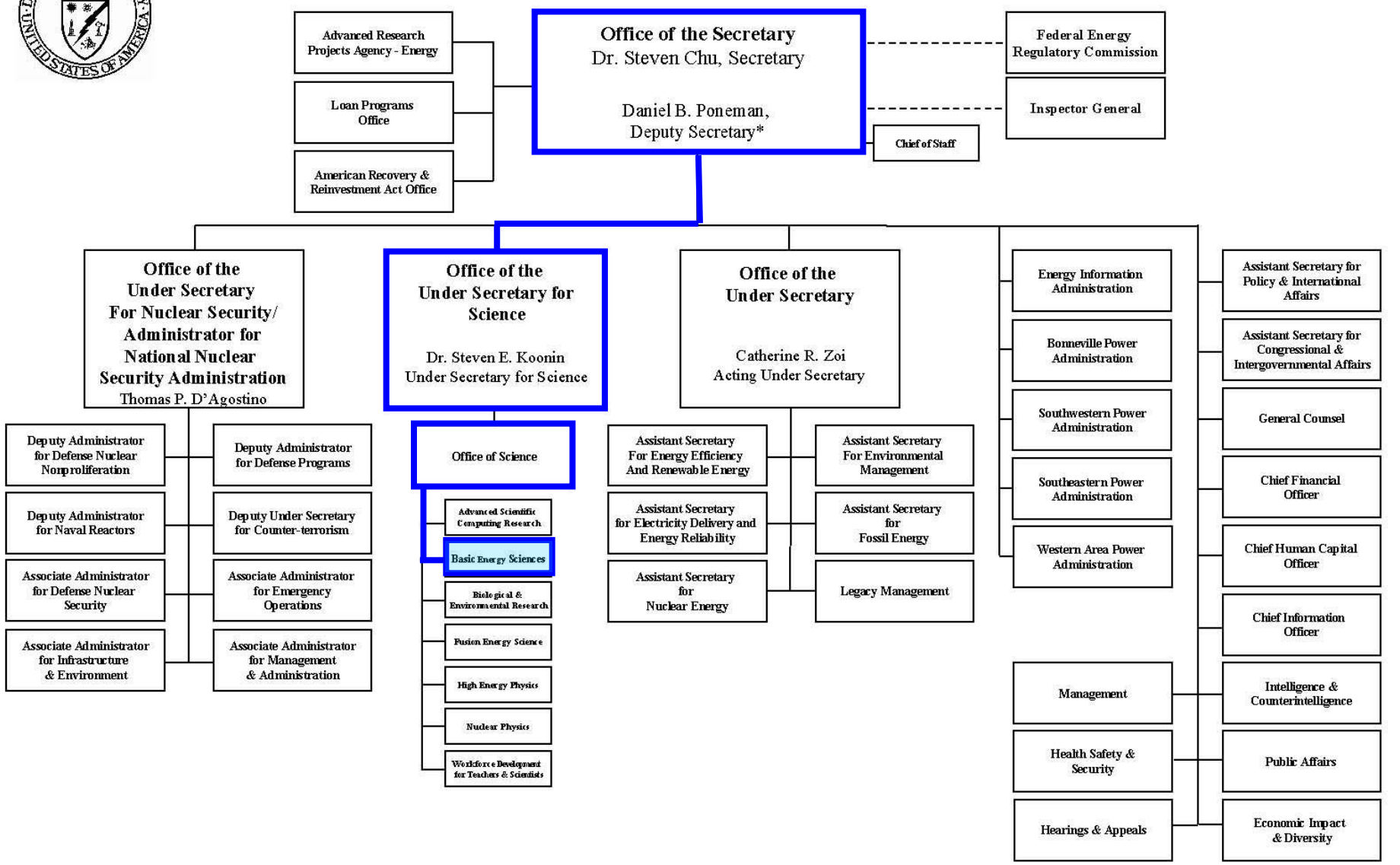
Office of Basic Energy Sciences
Office of Science

U.S. Department of Energy

Spring 2011 Meeting, Condensed Matter and Materials Research Committee (CMMRC) of the Board on Physics and Astronomy of the National Academies

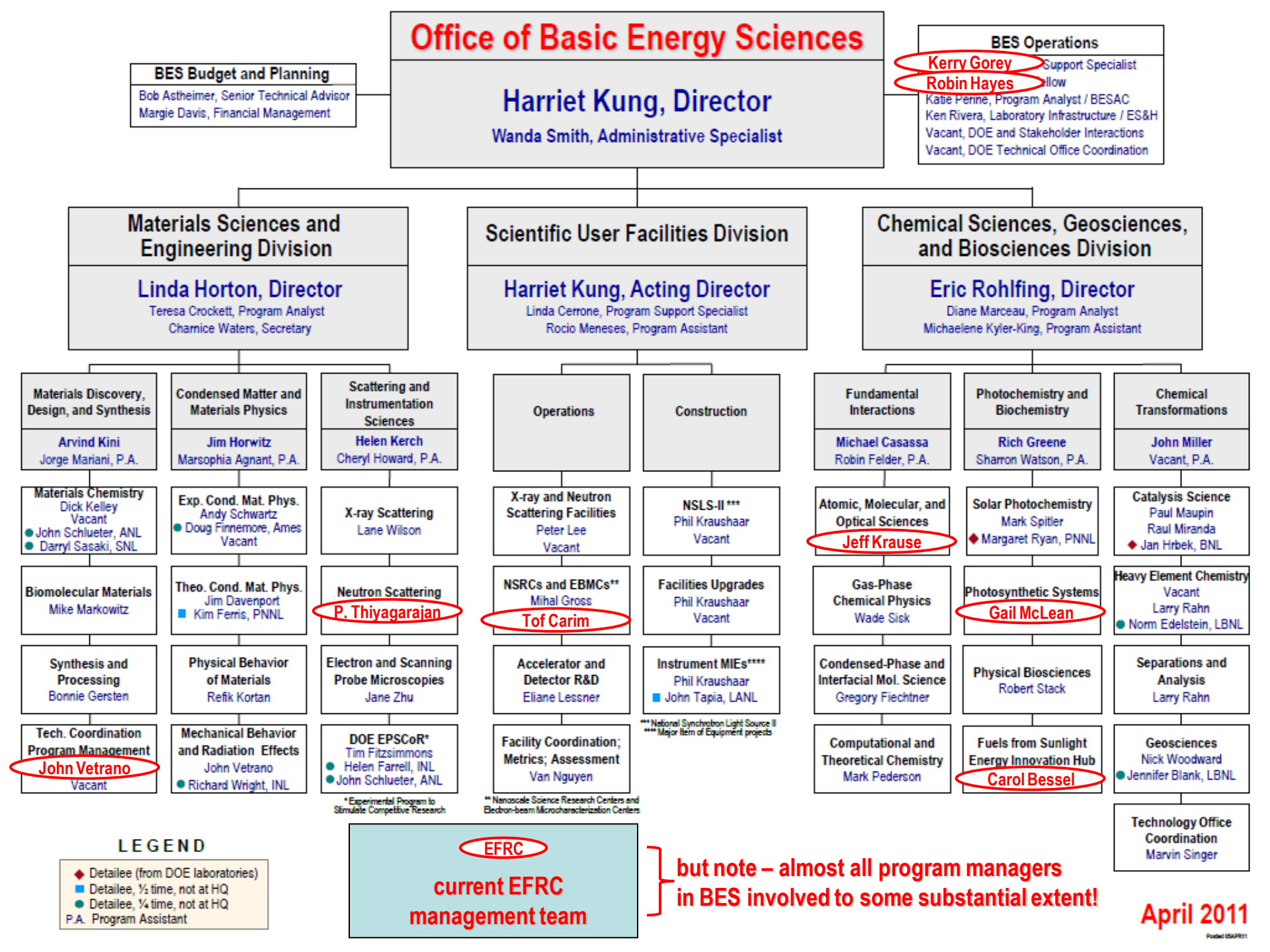
May 2, 2011 *Washington, DC*

DEPARTMENT OF ENERGY



* The Deputy Secretary also serves as the Chief Operating Officer

13 Oct 10


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
Kerry Gorey
Support Specialist
Robin Hayes
llow
Katie Perine, Program Analyst / BESAC
Ken Rivera, Laboratory Infrastructure / ES&H
Vacant, DOE and Stakeholder Interactions
Vacant, DOE Technical Office Coordination
Materials Sciences and Engineering Division
Linda Horton, Director
Teresa Crockett, Program Analyst
Charnice Waters, Secretary
Scientific User Facilities Division
Harriet Kung, Acting Director
Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant
Chemical Sciences, Geosciences, and Biosciences Division
Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant
Materials Discovery, Design, and Synthesis
Arvind Kini
Jorge Mariani, P.A.
Materials Chemistry
Dick Kelley
Vacant
John Schlueter, ANL
Darryl Sasaki, SNL
Biomolecular Materials
Mike Markowitz
Synthesis and Processing
Bonnie Gersten
Tech. Coordination Program Management
John Vetrano
Vacant
Condensed Matter and Materials Physics
Jim Horwitz
Marsophia Agnant, P.A.
Exp. Cond. Mat. Phys.
Andy Schwartz
Doug Finnemore, Ames
Vacant
Theo. Cond. Mat. Phys.
Jim Davenport
Kim Ferris, PNNL
Physical Behavior of Materials
Refik Kortan
Mechanical Behavior and Radiation Effects
John Vetrano
Richard Wright, INL
Scattering and Instrumentation Sciences
Helen Kerch
Cheryl Howard, P.A.
X-ray Scattering
Lane Wilson
Neutron Scattering
P. Thiyagarajan
Electron and Scanning Probe Microscopies
Jane Zhu
DOE EPSCoR*
Tim Fitzsimmons
Helen Farrell, INL
John Schlueter, ANL
* Experimental Program to Stimulate Competitive Research
Operations
X-ray and Neutron Scattering Facilities
Peter Lee
Vacant
NSRCs and EBMCs**
Mihal Gross
Tof Carim
Accelerator and Detector R&D
Eliane Lessner
Facility Coordination; Metrics; Assessment
Van Nguyen
** Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers
Construction
NSLS-II ***
Phil Kraushaar
Vacant
Facilities Upgrades
Phil Kraushaar
Vacant
Instrument MIEs****
Phil Kraushaar
John Tapia, LANL
*** National Synchrotron Light Source II
**** Major Item of Equipment projects
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 Mol. 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
Heavy Element Chemistry
Vacant
Larry Rahn
Norm Edelstein, LBNL
Separations and Analysis
Larry Rahn
Geosciences
Nick Woodward
Jennifer Blank, LBNL
Technology Office Coordination
Marvin Singer
LEGEND
Detailee (from DOE laboratories)
Detailee, ½ time, not at HQ
Detailee, ¼ time, not at HQ
P.A. Program Assistant
EFRC
current EFRC management team
but note – almost all program managers in BES involved to some substantial extent!
April 2011

Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science

EFRC awards provide the recipients with $2-5 million/year over a five-year award period to pursue collaborative basic research that addresses both energy challenges and science grand challenges in areas including:

- Solar Energy Utilization
- Bio-Fuels
- Catalysis
- Energy Storage
- Geosciences for Waste and CO_2 Storage
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen
- Combustion
- Superconductivity
- Solid State Lighting

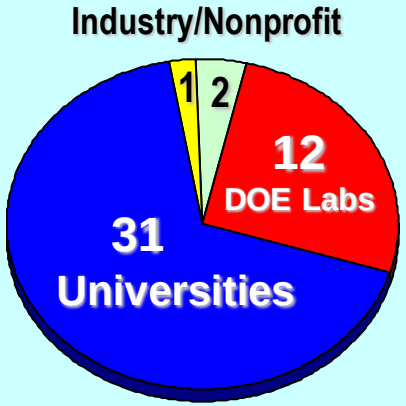
As stated in the original Funding Opportunity Announcement for the EFRCs:

"… the research proposed in the EFRC application must:

1) address one or more of the challenges described in the BESAC report Directing Matter and Energy: Five Challenges for Science and the Imagination, and

2) address one or more of the energy challenges described in the 10 BES workshop reports in the Basic Research Needs series"

A variety of lead institutions:



Total EFRCs = $777M over 5 years

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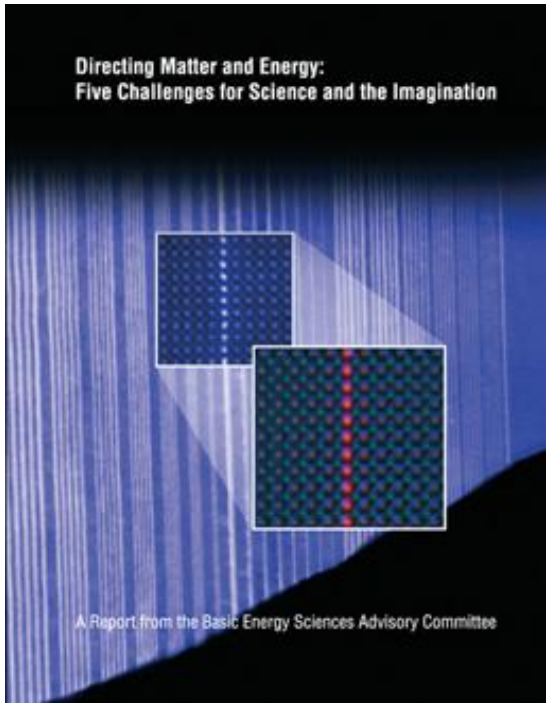
EFRCs: Addressing energy research challenges described in Basic Research Needs reports

In 2001, the Basic Energy Sciences Advisory Committee (BESAC) conducted a far reaching study leading to a comprehensive report, Basic Research Needs to Assure a Secure Energy Future. That report inspired a series of ten follow-on "Basic Research Needs" workshops and corresponding reports over the subsequent years, in coordination with the Department's technology offices, which together attracted more than 1,500 participants from universities, industry, and DOE laboratories and identified high priority research directions with promise to address the most critical knowledge and energy technology gaps.
(http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/)

EFRCs: Addressing the grand science challenges underpinning energy research

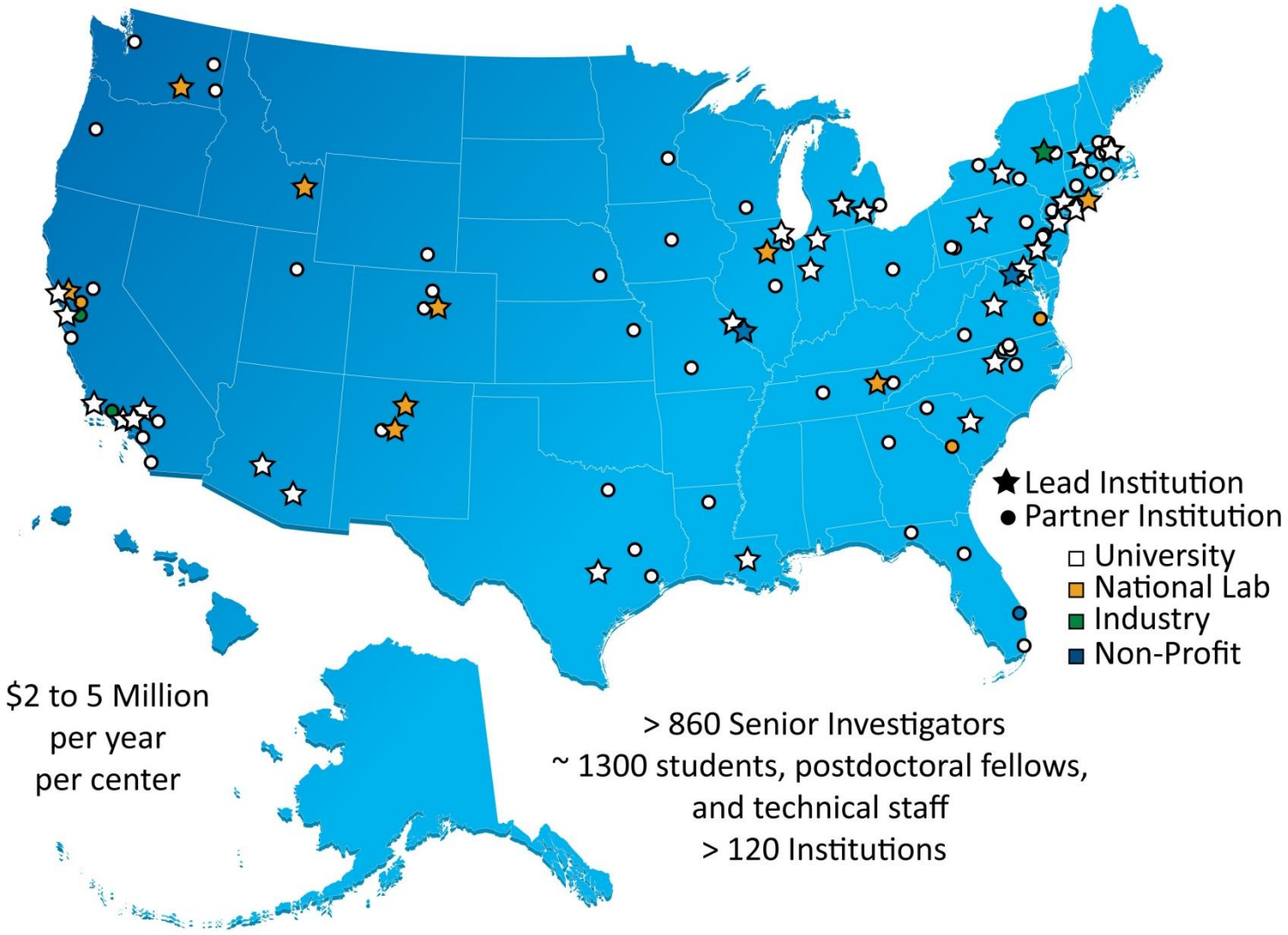
Roadblocks to progress and the opportunities for truly transformational new understanding were summarized in a BESAC report, Directing Matter and Energy: Five Challenges for Science and the Imagination:

- **How do we control materials processes at the level of electrons?**
- **How do we design and perfect atom- and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?**
- **How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?**
- **How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?**
- **How do we characterize and control matter away—especially very far away—from equilibrium?**



(http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/)

46 EFRCs established in August 2009, involving 35 States and DC



Roll call….

Center for Bio-Inspired Solar Fuel Production
Devens Gust, Arizona State University

Center for Interface Science: Solar Electric Materials
Neal R. Armstrong, University of Arizona

Center for Energy Efficient Materials
John Bowers, University of California, Santa Barbara

Center for Energy Nanoscience
P. Daniel Dapkus, University of Southern California

Center for Gas Separations Relevant to Clean Energy Technologies
Berend Smit, University of California, Berkeley

Center for Nanoscale Control of Geologic CO_2
Donald J. DePaolo, Lawrence Berkeley National Laboratory

Center on Nanostructuring for Efficient Energy Conversion
Fritz Prinz and Stacey Bent, Stanford University

Light-Material Interactions in Energy Conversion
Harry Atwater, California Institute of Technology

Molecularly Engineered Energy Materials
Vidvuds Ozolins, University of California, Los Angeles

Center for Inverse Design
Alex Zunger, National Renewable Energy Laboratory

Catalysis Center for Energy Innovation

Solid-State Solar-Thermal Energy Conversion Center
Gang Chen, Massachusetts Institute of Technology

Center for Solar and Thermal Energy Conversion
Peter F. Green, University of Michigan

Revolutionary Materials for Solid State Energy Conversion
Donald T. Morelli, Michigan State University

Center for Advanced Biofuel Systems
Richard T. Sayre, Donald Danforth Plant Science Center

Photosynthetic Antenna Frontier Research Center
Robert E. Blankenship, Washington University in St. Louis

Combustion Energy Frontier Research Center
Chung K. Law, Princeton University

Center for Advanced Solar Photophysics
Victor I. Klimov, Los Alamos National Laboratory

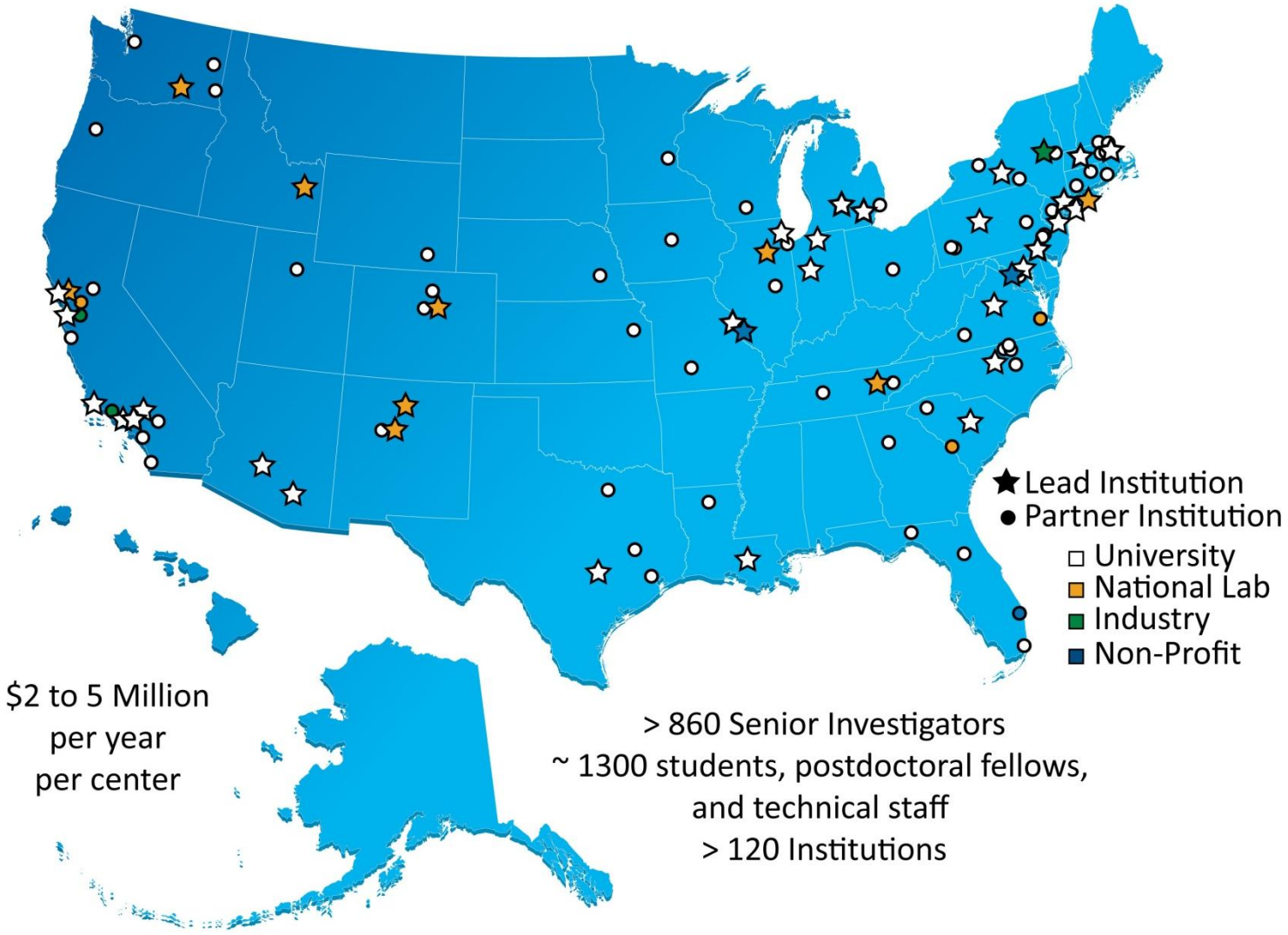
Center for Materials at Irradiation and Mechanical Extremes
Michael Nastasi, Los Alamos National Laboratory

EFRC for Solid State Lighting Science
Jerry A. Simmons, Sandia National Laboratories

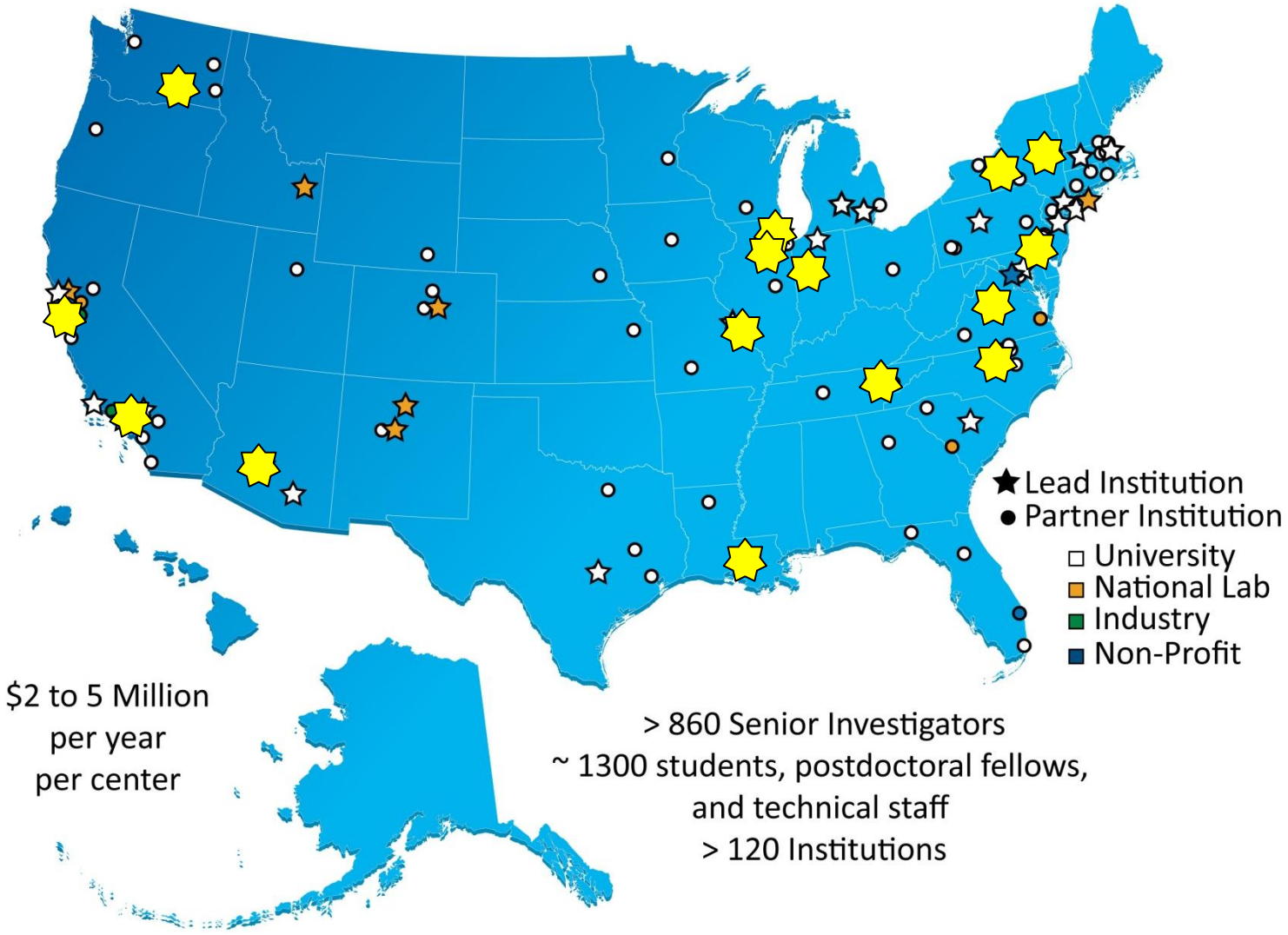
Center for Electrocatalysis, Transport Phenomena and Materials for Innovative Energy Storage
Grigorii Soloveichik, General Electric Global Research

Center for Emergent Superconductivity
J. C. Seamus Davis, Brookhaven National Laboratory

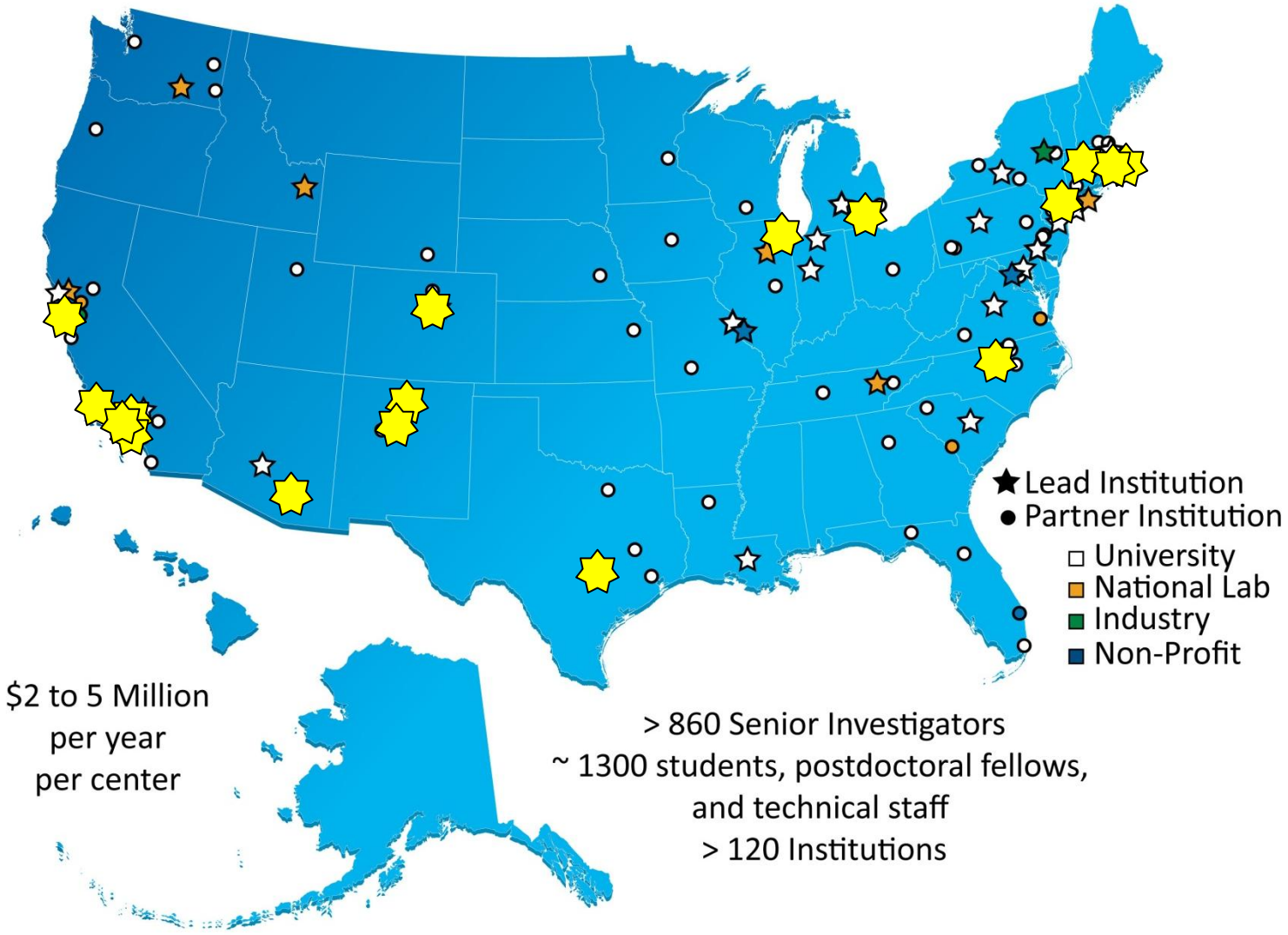
Better to consider areas of EFRC activity and impact than separate categories



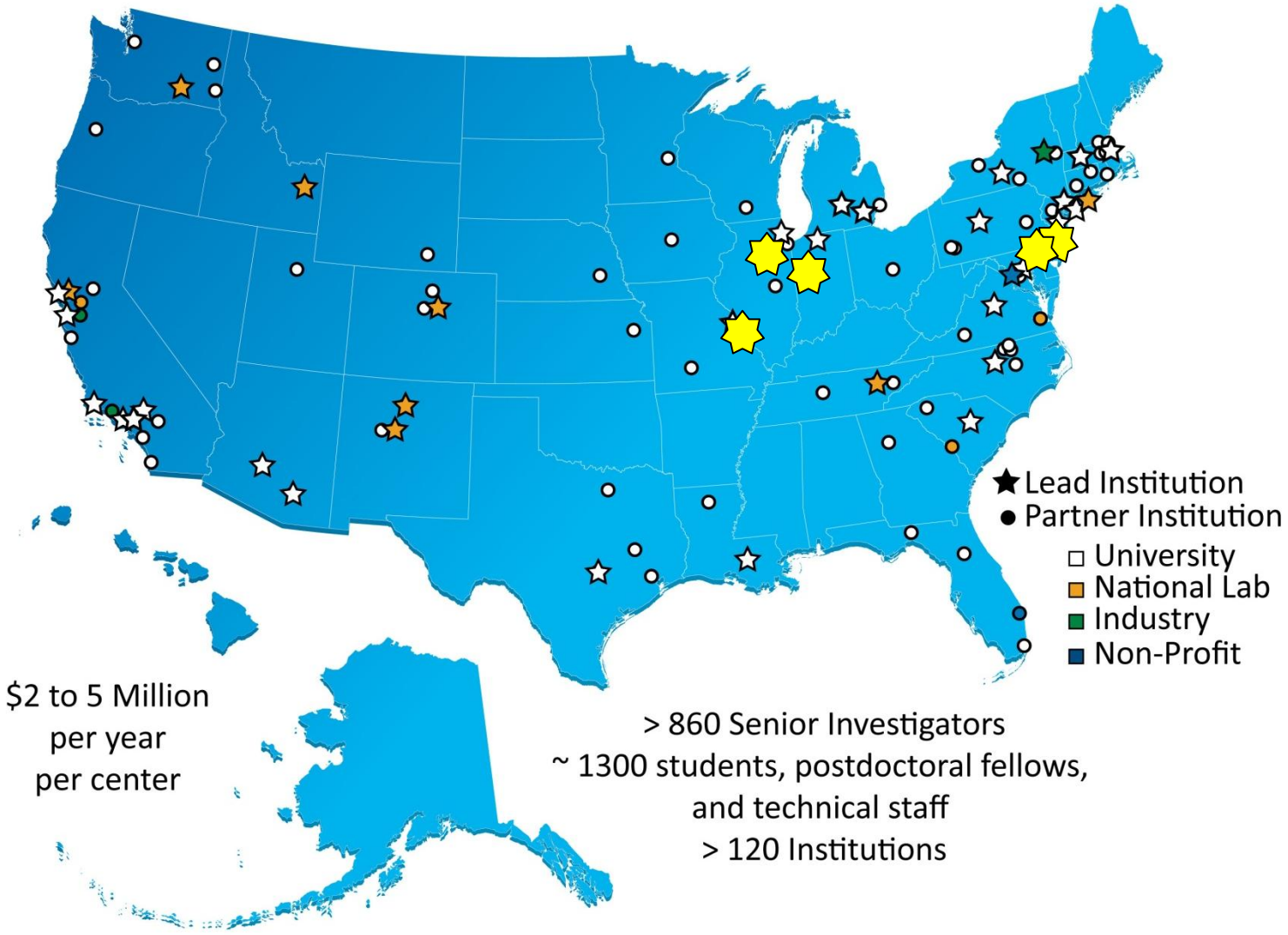
EFRCs with substantial activity in…..
Catalysis



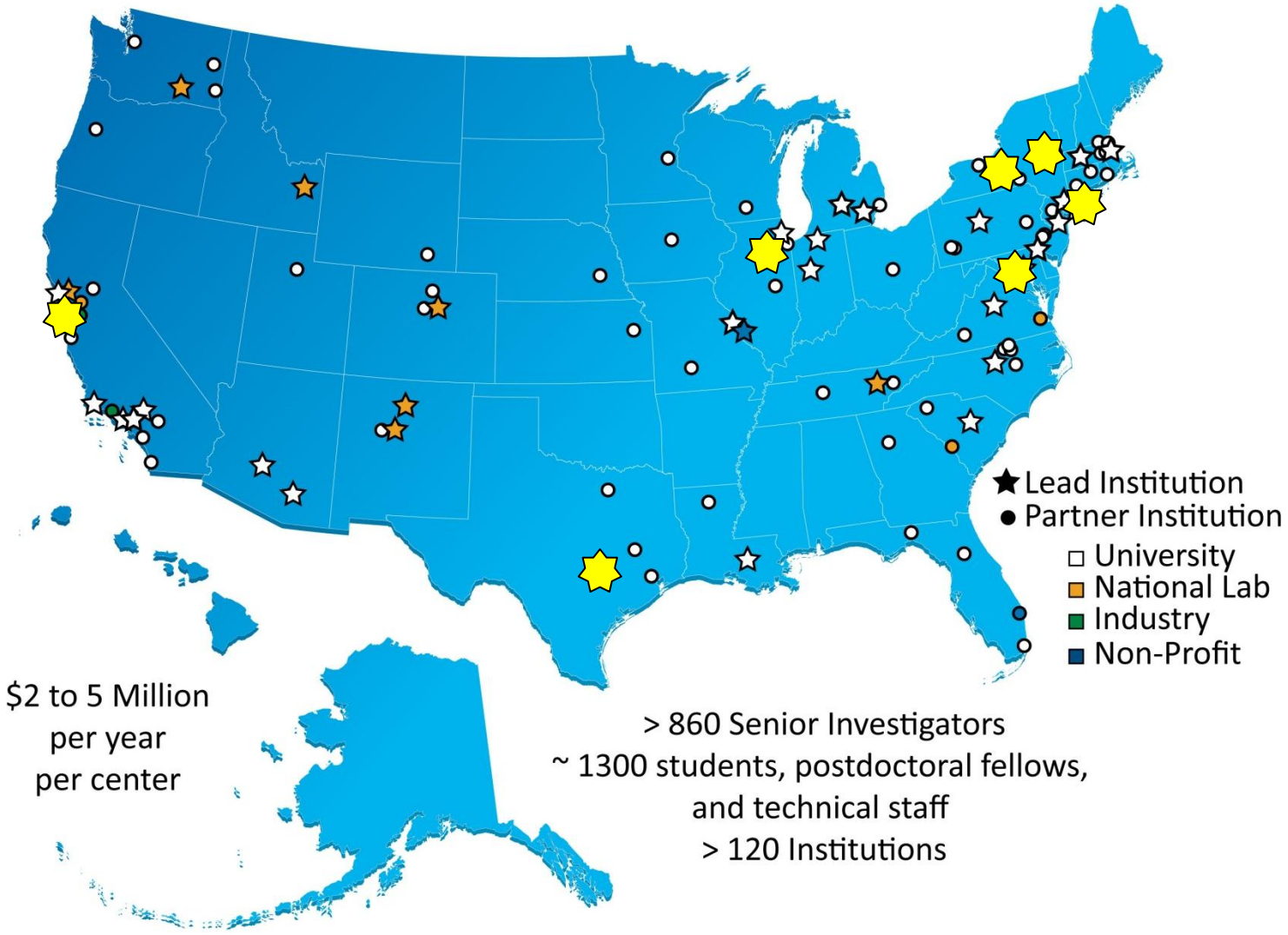
EFRCs with substantial activity in…..
Photovoltaics



EFRCs with substantial activity in…..
Biofuels



EFRCs with substantial activity in…..
Batteries



Single-slide synopsis of each EFRC

Center for Science of Precision Multifunctional Nanostructures for Electrical Energy Storage

Gary Rubloff (University of Maryland)

The EFRC will pursue multifunctional nanostructures as the basi
next generation of high per
electrical energy storage to

- power electric vehicles ov distances and recharge qu
- capture, hold, and deliver from renewable sources.

EFRC features:

- Metal oxide and silicon nan
- Carbon-nanowire composit structural stability during ch
- Fundamental understandin electrochemical behavior, s
- Uniform, predictable structu massive arrays in future tec

Sandia National Laboratories

Center for Frontiers of Subsurface Energy Security

Gary A. Pope (The University of Texas)

Summary statement: Our goal is scientific understanding of subsurface chemical and biological proce small to very large scale so th predict the behavior of CO_2 a byproducts of energy produc need to be stored in the subs

RESEAR

- Challenges and approache subsurface phenomena acr and modeling approaches t from equilibrium.
- Unique aspects: The uncer from the molecular scale to
- Outcome: Better understan

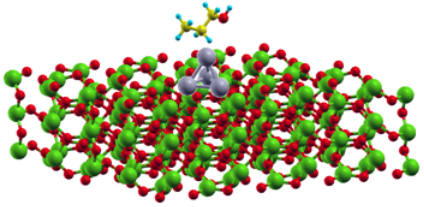
TEXAS

Sandia National Laboratories

Institute for Atom-efficient Chemical Transformations

Christopher L. Marshall (Argonne National Laboratory)

Summary statement: The *Institute for Atom-efficient Chemical Transformations (IACT)* a collaboration between Argonne National Laboratory, Northwestern University, University of Wisconsin and Purdue University is focused on advancing the *science* of catalysis for the efficient conversion of energy resources into usable forms.



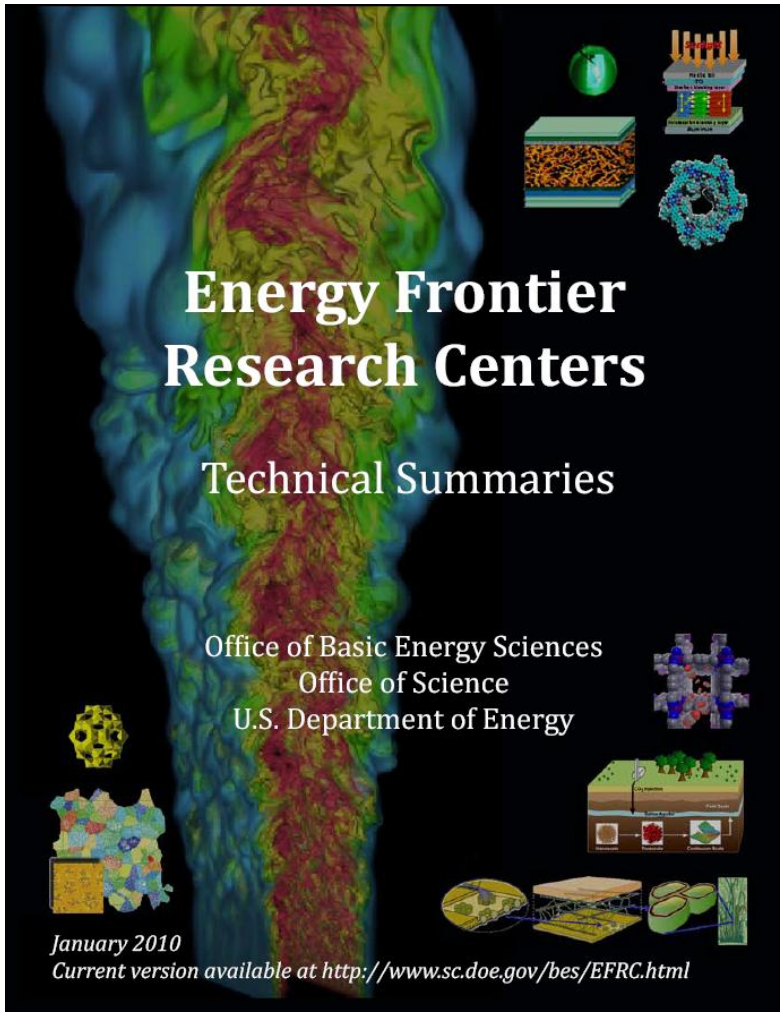
RESEARCH PLAN AND DIRECTIONS

Using a multidisciplinary approach involving integrated catalyst synthesis, advanced characterization, catalytic experimentation, and computation, IACT will address the key chemistries for the efficient removal of oxygen and hydrogen addition associated with the utilization of two primary energy resources in the United States, namely coal and biomass.

Argonne NATIONAL LABORATORY | NORTHWESTERN UNIVERSITY | THE UNIVERSITY OF WISCONSIN MADISON | PURDUE UNIVERSITY

an Office of Basic Energy Sciences Energy Frontier Research Center

Technical summaries book



Two-page technical summaries were provided and updated by EFRCs in the latter half of calendar 2009, and were compiled and made broadly available in early 2010

New updates submitted recently and will be made available as a revised document soon

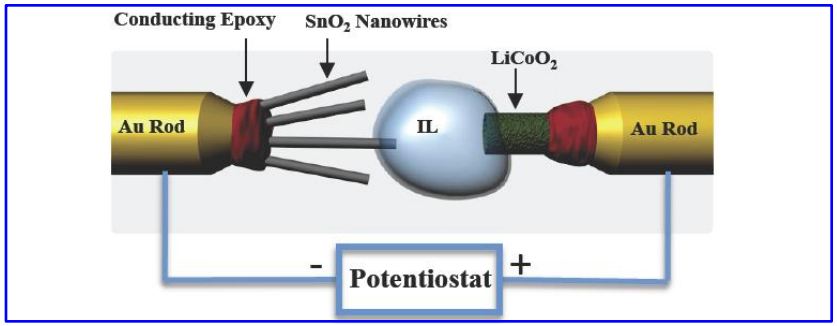
Includes EFRC contact information and indexing by:

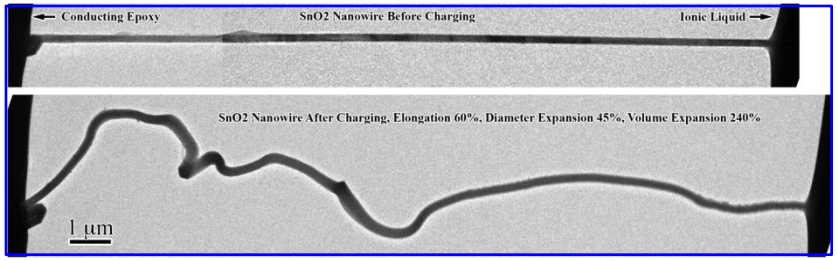
- **Investigator**
- **Institution**
- **Basic Research Needs**
- **Grand Challenges**
- **Topical Keywords**
- **Experimental and Theoretical Methods**

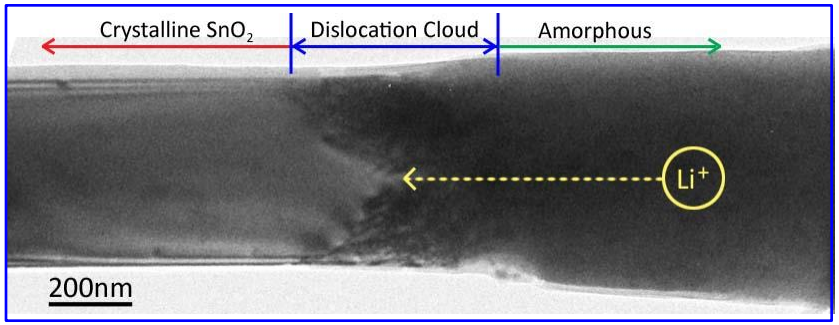
Real-time Imaging of Nano-Battery Operation

Evolution of single-nanowire electrode in Li-ion battery

- **World's smallest battery inside a transmission electron microscope enables real time observations of electrochemistry processes at atomistic length scales**
- **A unique open cell battery using ionic liquid electrolyte in the high vacuum of a TEM**
- **New insight into electrochemical processes critical to developing new high performance batteries**
  - **Nanowires can sustain large stresses (>10 GPa) caused by Li^+ transport without breaking, good candidate for battery**
  - **Elongation and twisting of nanowires during charging may lead to a short circuit and failure of the battery, a key factor to consider during design**







Jian Yu Huang, et al., *Science 330, 1515 (2010)*

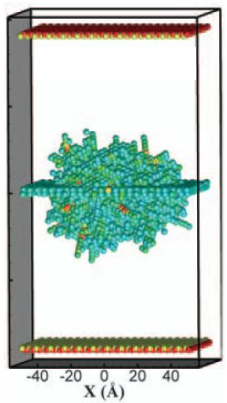
- Research at Sandia National Laboratory supported by the *Center for Science of Precision Multifunctional Nano-structures for Electrical Energy Storage* (an EFRC led by University of Maryland), and in collaboration with Pacific Northwest National Laboratory and university contributors

Improvements in Radiation Damage Tolerance

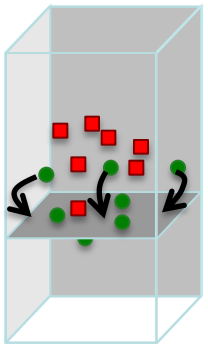
Simulations reveal unexpected self-healing mechanism

- **Simulations reveal why nanostructured materials with a large number of grain boundaries exhibit increased tolerance to radiation damage**
- **New interstitial emission and vacancy recombination mechanism critical to self-healing of radiation damaged material**
  - **At very short times, interstitial atoms are concentrated on the grain boundary, but at longer times they re-emit and annihilate trapped vacancies many atomic distances away**
  - **Grain boundaries loaded with interstitials reduce the barrier for vacancy diffusion and promote defect recombination**
  - **Designed nanostructured grain boundaries could slow down the accumulation of radiation damage**

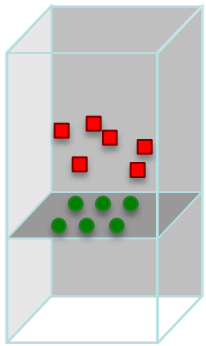
- **Research supported by the *Center for Materials at Irradiation and Mechanical Extremes* (an EFRC led by Los Alamos National Laboratory)**



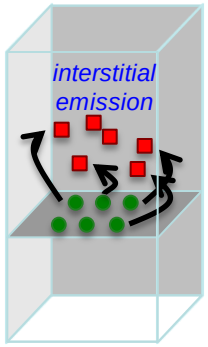
Radiation damage



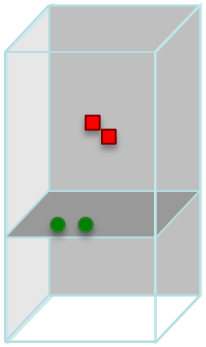
Interstitials quickly move to grain boundary



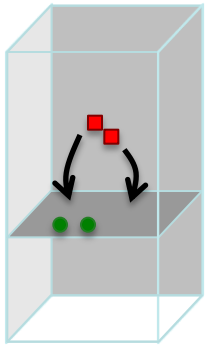
Vacancies trapped in bulk material



Interstitials emit from grain boundary



Interstitials and vacancies recombine

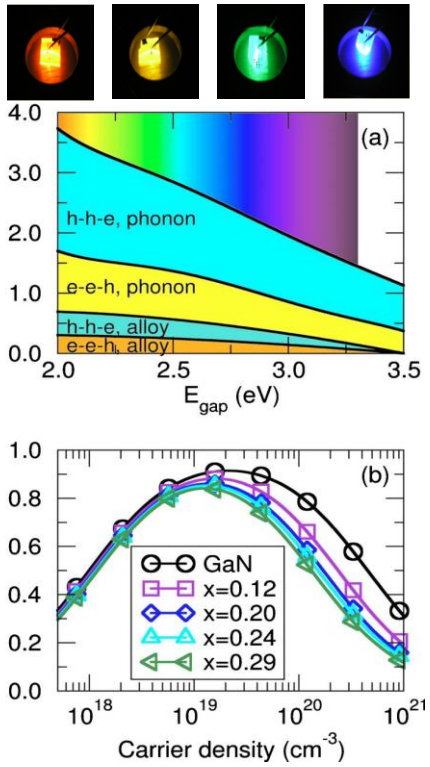


Diffusion of remaining vacancies very slow

Xian-Ming Bai et al. *Science, 327, 1631 (2010)*

Understanding Efficiency "Droop" in LEDs

Identifying origins could have impacts on solid-state lighting



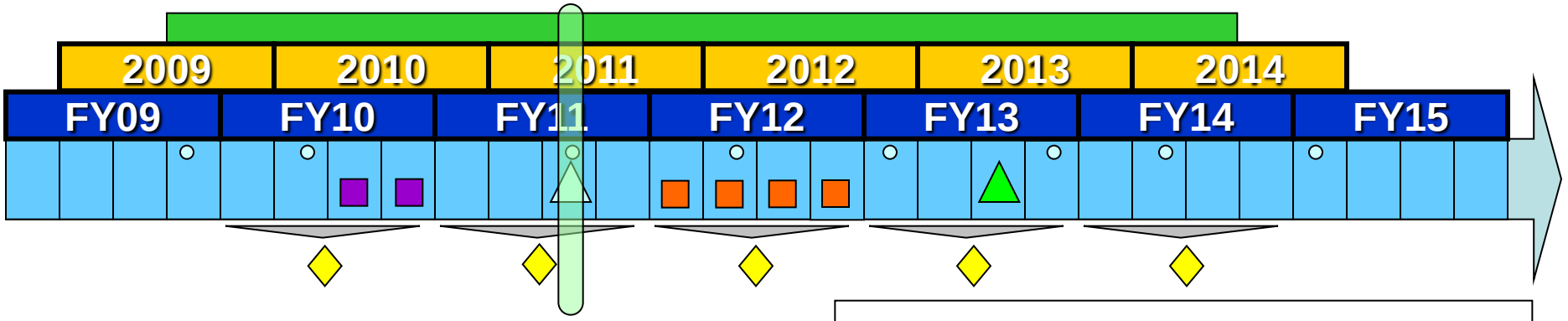
Upper Figures: **Images of LEDs.**
Middle Figure: **Phonon mediated processes substantially affect Auger coefficient in InGaN.**
Lower Figure: **Droop in efficiency occurs at high carrier densities in InGaN alloys, and worsens at higher indium content (x).**

- **The cause of "droop" in light-emitting diodes (LEDs) – a drop-off in efficiency at high current levels – has been unresolved for years.**
  - **Increasing the input current does not produce a proportional increase in the light output of an LED, thus LED efficiency at high power is less than the efficiency at low operating power.**
- **New atomistic first-principles calculations demonstrate that droop in (In)GaN-based LEDs is consistent with an indirect Auger recombination process.**
  - **Electron-phonon coupling and alloy scattering (breaking of symmetry due to insertion of indium) substantially increases the likelihood of detrimental Auger transitions.**
  - **Since the Auger process involves three charged particles, this mechanism becomes more prominent at high current injection levels.**
  - **By identifying origins of droop, this result provides a guide to addressing the efficiency issues in nitride LEDs and the development of more efficient solid-state lighting**
- **Research supported by the *Center for Energy Efficient Materials* (an EFRC led by UC Santa Barbara**

E. Kioupakis, et al., *Applied Physics Letters* 2011, 98, 161107.

UCSB | NREL National Renewable Energy Laboratory | Los Alamos National Laboratory | UC Santa Cruz | Harvard

EFRCs Management Timeline



COMMUNICATION:

- DOE and individual EFRC web sites established
- Monthly management conference calls (by topical groups)
- Periodic Directors' meetings
- Informal site visits by BES
- EFRCs Summit and Forum (FY11, 3rd Quarter, in DC)
- Energy Frontiers workshop (FY13, tentatively 3rd Quarter)
- BES Contractors' meetings, by topic

REVIEW SCHEDULE:

- Initial reverse site management/operations review – FY10 3rd/4th Quarter
- Interim science and management review – FY12

- Initial Award Period
- Periodic Directors' Meeting (tied to alternate BESAC meetings)
- Reverse Site Peer Reviews (Management/Operations focus)
- In-Depth Peer Reviews (Science focus)
- EFRCs Summit and Forum
- Energy Frontiers Workshop
- BES Topical Contractors Meetings (as appropriate)

EFRCs are grouped for management purposes

Monthly teleconferences by EFRC subgroups; these have evolved from largely administrative discussions to having more science content and discussion.

Indigo (*new MSE hire; Thiyaga/Vetrano for now*)

M. Baldo – MIT
G. Chen – MIT
P. Green – Michigan
B. Grzybowski – Northwestern
D. Dapkus – USC
S. Davis – BNL
C. Grey – Stony Brook
G. Rubloff – Maryland
J. Simmons – SNL
M. Thackeray – ANL
D. Wesolowski – ORNL
J. Yardley – Columbia

Red (Vetrano)

T. Allen – INL
P. Burns – Notre Dame
H.-K. Mao – Carnegie
M. Nastasi – LANL
M. Stocks – ORNL

Blue (Thiyaga)

D. DePaolo – LBNL
D. Morelli – MI State
V. Ozolins – UCLA
G. Pope – UT Austin
B. Smit – UC Berkeley
A. Zunger – NREL

Yellow (Bessel)

H. Abruña – Cornell
N. Armstrong – Arizona
H. Atwater – Caltech
J. Bowers – UCSB
M. Bullock – PNNL
D. Gust – ASU
V. Klimov – LANL
T. Meyer – UNC
F. Prinz/S. Bent – Stanford
K. Reifsnider – S Carolina
T. Russell and P. Lahti – U Mass
M. Wasielewski – Northwestern

Orange (McLean)

R. Blankenship – Washington U.
D. Cosgrove – PSU
C. Law – Princeton
M. McCann – Purdue
R. Sayre – Danforth Plant Science Center

Violet (Krause)

B. Gunnoe – U. Va.
C. Marshall – ANL
G. Soloveichik – GE
J. Spivey – LSU
D. Vlachos – Delaware
X. Zhu – UT Austin

Other BES program managers also participate

December 2010

Management Reference Documents

Intended to be compact (1 or 2 page) guidelines for various aspects of EFRC operations and interactions with BES; issued as needed.

Acknowledgements

- **Covers crediting and delineation in papers, presentations, press releases**

Annual Progress Reports

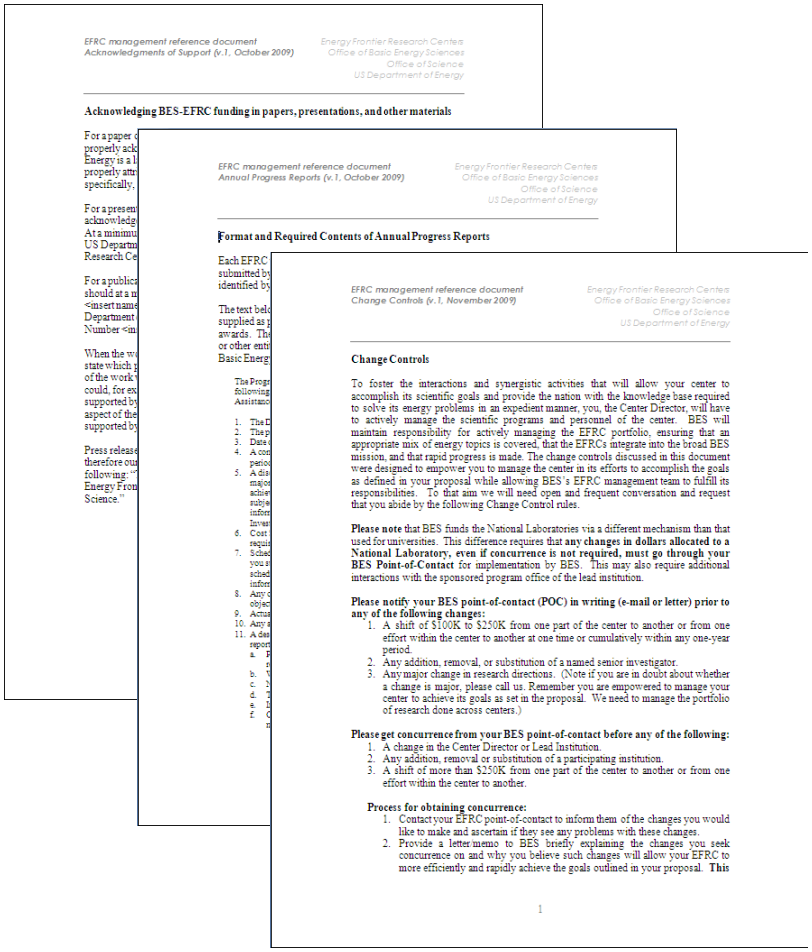
- **Uniform annual reporting structure, including spreadsheet template for staffing information**

Change Controls

- **Outlines parameters of EFRC changes requiring notification or concurrence**

Expectations and Good Practices

- **Summarizes lessons learned from initial management reviews in 2010**



EFRC management reference document
Acknowledgments of Support (v.1, October 2009)

Energy Frontier Research Centers
Office of Basic Energy Sciences
Office of Science
US Department of Energy

Acknowledging BES-EFRC funding in papers, presentations, and other materials

EFRC management reference document
Annual Progress Reports (v.1, October 2009)

Energy Frontier Research Centers
Office of Basic Energy Sciences
Office of Science
US Department of Energy

Format and Required Contents of Annual Progress Reports

EFRC management reference document
Change Controls (v.1, November 2009)

Energy Frontier Research Centers
Office of Basic Energy Sciences
Office of Science
US Department of Energy

Change Controls

To foster the interactions and synergistic activities that will allow your center to accomplish its scientific goals and provide the nation with the knowledge base required to solve its energy problems in an expedient manner, you, the Center Director, will have to actively manage the scientific programs and personnel of the center. BES will maintain responsibility for actively managing the EFRC portfolio, ensuring that an appropriate mix of energy topics is covered, that the EFRCs integrate into the broad BES mission, and that rapid progress is made. The change controls discussed in this document were designed to empower you to manage the center in its efforts to accomplish the goals as defined in your proposal while allowing BES's EFRC management team to fulfill its responsibilities. To that aim we will need open and frequent conversation and request that you abide by the following Change Control rules.

Please note that BES funds the National Laboratories via a different mechanism than that used for universities. This difference requires that **any changes in dollars allocated to a National Laboratory, even if concurrence is not required, must go through your BES Point-of-Contact** for implementation by BES. This may also require additional interactions with the sponsored program office of the lead institution.

Please notify your BES point-of-contact (POC) in writing (e-mail or letter) prior to any of the following changes:

1. A shift of $100K to $250K from one part of the center to another or from one effort within the center to another at one time or cumulatively within any one-year period.
2. Any addition, removal, or substitution of a named senior investigator.
3. Any major change in research directions. (Note if you are in doubt about whether a change is major, please call us. Remember you are empowered to manage your center to achieve its goals as set in the proposal. We need to manage the portfolio of research done across centers.)

Please get concurrence from your BES point-of-contact before any of the following:

1. A change in the Center Director or Lead Institution.
2. Any addition, removal or substitution of a participating institution.
3. A shift of more than $250K from one part of the center to another or from one effort within the center to another.

Process for obtaining concurrence:

1. Contact your EFRC point-of-contact to inform them of the changes you would like to make and ascertain if they see any problems with these changes.
2. Provide a letter/memo to BES briefly explaining the changes you seek concurrence on and why you believe such changes will allow your EFRC to more efficiently and rapidly achieve the goals outlined in your proposal. **This**

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May 25–27, 2011
Washington, D.C.

Renaissance Penn
Quarter Hotel

Science for our Nation's Energy Future

Energy Frontier Research Centers Summit & Forum

Transforming the future
of energy and
the environment.

www.energyfrontier.us

U.S. DEPARTMENT OF ENERGY | Office of Science

Science for our Nation's Energy Future
Energy Frontier Research Centers Summit & Forum

May 25–27, 2011
Washington, D.C.

Renaissance Penn Quarter Hotel

Science for Our Nation's Energy Future will:

- Explore the challenges and opportunities in applying America's extraordinary scientific and technical resources to critical energy needs
- Highlight early successes of the Office of Science Energy Frontier Research Centers
- Promote collaboration across the national energy enterprise

Expected Participants include:

- Leaders from science, industry and government from the US and abroad
- Students, young researchers, and senior investigators
- Members of the media and the general public
- Anticipated attendance on the order of 900-1200; no registration fee

Energy Frontier Research Centers Summit

May 25, 2011

Open to the public

Speakers include:

- **Steven Chu** – US Secretary of Energy
- **John Hennessy** – President of Stanford University
- **Mark Little** – Senior VP and Director of GE Global Research
- **Eric Isaacs** – Director of Argonne National Laboratory
- **Nate Lewis** – Director of JCAP, Fuels from Sunlight Energy Innovation Hub
- **Congressional Representatives**
- **Energy Frontier Research Center Senior Investigators**

Life at the Frontiers of Energy Research video competition award ceremony

Poster session and reception featuring the 46 Energy Frontier Research Centers

Science for our Nation's Energy Future
Energy Frontier Research Centers Summit & Forum

May 25–27, 2011
Washington, D.C.

Renaissance Penn Quarter Hotel

Energy Frontier Research Centers Forum

May 26-27, 2011

Open to the public

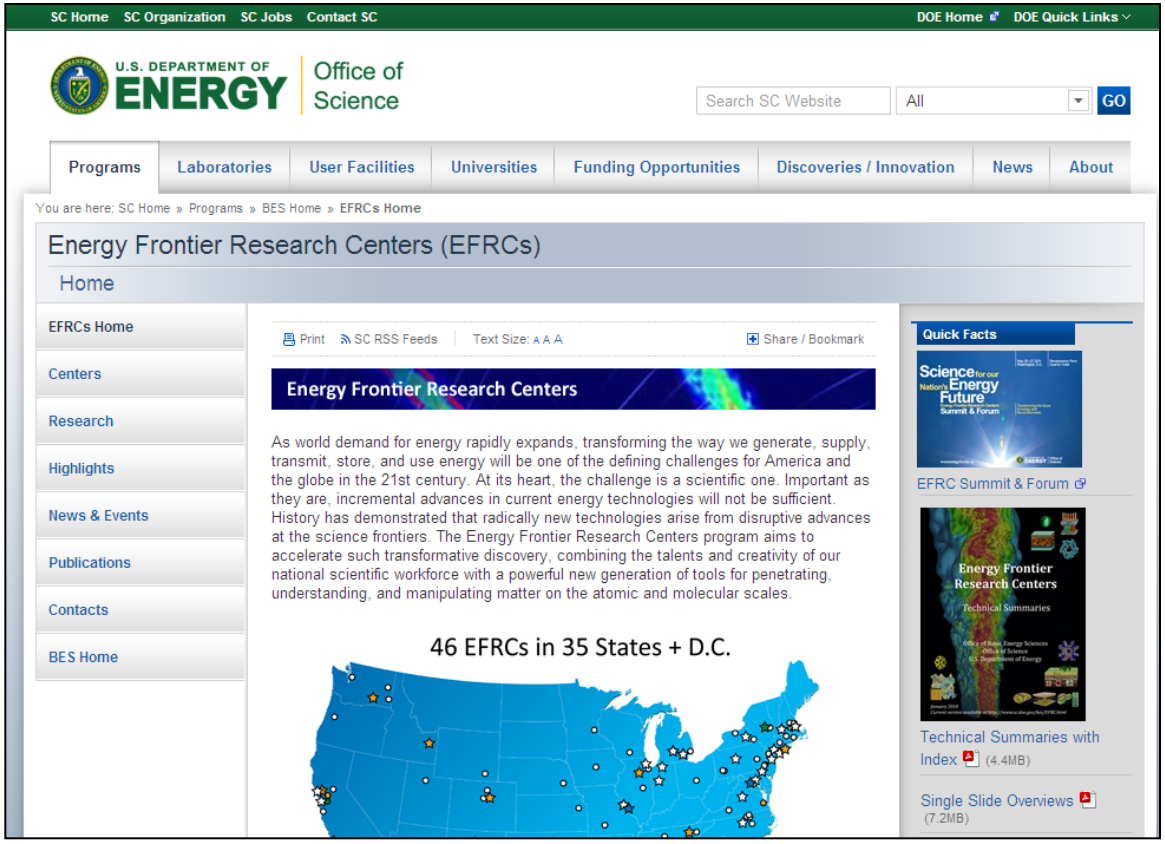
Keynote speakers, technical sessions, and poster presentations

Parallel Scientific Sessions include:

- Organic photovoltaics
- Inorganic photovoltaics
- Solar fuels and biomass
- Energy storage and transmission
- Energy conservation and efficiency
- Carbon capture and sequestration
- Materials in extreme environments
- Effective and sustainable materials design: integration of computation, theory and experiment
- New tools and methods for materials synthesis and characterization

EFRC web site has extensive information, links

- **Overall information about EFRC program**
- **Clickable map with links to individual summary pages for each EFRC**
- **Access to various documents including:**
  - **compilation of two-page EFRC technical summaries (with keyword indices)**
  - **Single-slide summaries**
  - **Q & A**
  - **fact sheet**
- **Budget information**



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

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