Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science

BESAC
07/07/15

http://www.besac2014.com/
From: Dr. Pat Dehmer (Acting Director of Office of Science)

The new BESAC study should evaluate the breakthrough potential of current and prospective energy science frontiers based on how well the research advances the five grand science challenges. Your report will advise BES in its future development of focused, effective research strategies for sustained U.S. leadership in science innovation and energy research.

I ask BESAC to consider the following questions in formulating the study plan:

- What progress has been achieved in our understanding of the five BESAC Grand Science Challenges?
- What impact has advancement in the five Grand Science Challenges had on addressing DOE’s energy missions? With evolving energy technology and U.S. energy landscape, what fundamental new knowledge areas are needed to further advance the energy sciences? Please consider examples where filling the knowledge gaps will have direct impacts on energy sciences.
- What should the balance of funding modalities (e.g., core research, EFRCs, Hubs) be for BES to fully capitalize on the emerging opportunities?
- Identify research areas that may not be sufficiently supported or represented in the US community to fully address the DOE’s missions.
BESAC Subcommittee on Challenges at the Frontiers of Matter and Energy

Subcommittee
Nora Berrah (University of Connecticut)
Gordon Brown (Stanford University)**
Susan Coppersmith (University of Wisconsin-Madison)
Don DePaolo (LBNL and University of California-Berkeley)
Roger French (Case Western Reserve University)**
Cynthia Friend (Harvard University)
Ian Foster (ANL and University of Chicago)
Sharon Glotzer (University of Michigan)
Bruce Kay (Pacific Northwest National Laboratory)**
Jennifer Lewis (Harvard University)
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Juan de Pablo (University of Chicago)
Tijana Rajh (Argonne National Laboratory)
Anthony Rollett (Carnegie Mellon University)**
Maria Santore (University of Massachusetts)**
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William Tumas (National Renewable Energy Laboratory)

Executive Committee
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George Crabtree (ANL & Univ. of Ill. at Chicago)
Mark Ratner (Northwestern)**
Graham Fleming (UC Berkeley)
John Hemminger, ex-officio (UC-Irvine)*

Thanks to
Lynn Yarris, Science Writer, LBNL
Natalia Melcer, BES
ANL Editorial & Production Team

*BESAC Chair
**BESAC Member
The Subcommittee gathered broad input from the community

- **Subcommittee meetings**
  - Bethesda, 7/31 & 8/1; kick-off workshop
  - Berkeley, 8/28 & 8/29; focus on computing and correlated matter
  - Evanston, 10/21 & 10/22; focus on synthesis and soft matter
  - Cambridge, 12/4 & 12/5; focus on gas phase chemistry
  - Germantown, 1/14 & 1/15; initial red team review of message/report

- **Community input at** [www.besac2014.com](http://www.besac2014.com)
  - Targeted appeal to EFRC Directors and Early Career Awardees

- **We’ve continued to listen**
  - Townhall: APS March Meeting, March 4, 2015
Takeaways from February BESAC meeting

• BESAC approved Transformative Opportunities
• Generally correct elements to “Enable Success”
  – Distill to critical few

• Several topical themes needed tightening
  – Strength/clarity of non-soft matter synthesis discussion
  – Breadth of coherence opportunity
  – Ensure “chemistry voice” present
  – “Acceleration” as a missing theme (not just ‘why’ but ‘why now’)

• Report mechanics to address
  – Placement of “Chapter 5 – Grand Challenges: Then and Now”
  – Complete/ensure diversity of sidebars
  – Strive for “Scientific American” throughout; reduce/eliminate jargon/cliches
Plan for This Meeting

- Tuesday am (this talk): Review of the report’s message and how it’s captured in the printed document
- Tuesday pm: BESAC discussion/detailed feedback on open issues needing attention
- Wednesday am: Our plan of attack for responding to your feedback & sending the report to press asap

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Remember 2007…

- At least some of us were much younger
- We were actively working Basic Research Needs for xxx
- EFRCs did not exist
- SC Early Career Awards did not exist
- Lots of compelling research had not yet occurred
- NSLS-II, LCLS were visions, NOT working facilities
- Petascale computing was a goal, not a reality
The 2007 Grand Challenges are still compelling AND the landscape has changed as a result of our progress

How Do We Control Material Processes at the Level of Electrons?

How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?

How do remarkable properties of matter emerge from complex correlations of the 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?
In the report, continued opportunity is highlighted in Introduction and details are discussed in “Grand Challenges: Then and Now”

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Advances in data, algorithms & computing, and imaging across scales will, with strategic investments, further accelerate future progress.
How Do We Control Material Processes at the Level of Electrons?

Much of the last century has focused on understanding how electrons in matter – their charge, their spin, and their dynamics – determine the properties of materials and how they direct chemical, electrical, or physical processes in materials. We are now on the verge of a new science of quantum control where our tools will go beyond probing what is there, towards the goal of controlling these processes and properties through direct manipulation of the electrons.

Controlling materials processes at the level of electrons has an enormously wide horizon. The broader challenges in single layer, soft, amorphous and heterogeneous materials that enable the remarkable functionality of biology and promise to bring similar complexity and functionality to artificial energy materials remain to be explored.
How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?

The periodic table contains more than 110 elements, but only a tiny fraction of all possible chemical compounds has yet been prepared and their properties characterized. Moving beyond trial-and-error searching, science is in favorable cases now approaching the threshold of ‘directed’ synthesis guided by predictive design, based on first-principles, of materials with properties that we desire.

Directed Self-Assembly

Materials Genome

In situ characterization

Innovation and resources are needed for synthesis and characterization to reach a level commensurate with predictive materials by design, allowing all three activities—discovery, synthesis and characterization—to work collaboratively to advance our collective materials wisdom.
How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?

Emergent phenomena, in which the correlated behavior of many atomic or electronic constituents leads to an unexpected collective outcome, are of great significance across the sciences and engineering. Uncovering the fundamental rules of correlations and emergence is the first part of the challenge. The second is to achieve control over these correlations, a prospect that can only now be reasonably contemplated with the advent of tools to probe and affect particles and their correlations on the nanoscale. By understanding and controlling correlations, we can put emergences to work for us.

Correlation and the emergence of the new phenomena it drives are wellsprings of scientific discovery and innovation, ripe for the harnessing of new functionalities and applications.
How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?

Implementation and utilization of complex nanotechnologies with capabilities approaching those found within the biological world remains beyond our reach at present. The ways in which energy, entropy, and information are manipulated within living nanosystems provide us with lessons on what humans must learn to do in order to develop similarly sophisticated technologies.

Folding Polymers

Molecular Motors

Self-Regulation

As we develop the tools to unravel biology’s most important secrets and remarkable successes in harnessing complexity for functionality, we can look forward to equally rich and expansive achievements in applying biology’s lessons to artificial energy materials, and even ultimately exceeding biology’s capabilities.
How do we characterize and control matter away - especially very far away - from equilibrium?

At equilibrium, we can make many significant statements about what can happen, about the states of matter and of energy, and about the structures that occur. The same is not true when we consider systems out of equilibrium, a state in which much of Nature finds itself much of the time. Understanding non-equilibrium processes and systems requires addressing the major difficulties associated with bridging theories across many length and time scales in order to construct meaningful statements and organizing principles to describe Nature most completely over the many relevant scales of time and of size.

Critical universal questions remain:

By what mechanisms and how fast do far-from-equilibrium systems evolve?
Are there barriers to reaching equilibrium, or metastable states in which to trap the system?
How can we harness or manipulate transformations driven by disequilibrium?
Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science

Instrumentation & Tools

Human Capital

Synthesis

Mastering Hierarchical Architectures

Beyond Ideal Materials and Systems

Harnessing Coherence in Light and Matter

Data, Algorithms and Computing

Efficient Synthesis for Tailored Properties

Energy and Information on the Nanoscale

Correlated Systems

Control at the Level of Electrons

Imaging Matter across Scales

Systems Away from Equilibrium
New Transformative Opportunities have emerged that have their foundations in the Grand Challenges

“The most exciting phrase to hear in science, the one that heralds new discoveries, is not ‘Eureka!’ but ‘That's funny...’” —Isaac Asimov

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

Crosscutting Opportunities

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

Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales
Mastering Hierarchical Architectures and Beyond-Equilibrium Matter

The transformative opportunity is to realize targeted functionality in materials by controlling the synthesis and assembly of hierarchical architectures and beyond-equilibrium matter, thereby increasing dramatically the exploration space for enhanced function.

To realize this opportunity, several major advances are required:

1) predictive models, including the incorporation of metastability, to guide the creation of beyond equilibrium matter
2) Mastering synthesis and assembly of hierarchical structures for multi-dimensional hybrid matter
3) \textit{in situ} characterization of spatial and temporal evolution during their synthesis and assembly
Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces and Disorder

Developing a fundamental understanding of the roles of heterogeneities, interfacial processes, and disorder in materials behavior represents a transformative opportunity to move from ideal systems to the complexity of real systems under realistic conditions.

- Science of scale
- Slow and statistically rare events
- “epidemiological” studies of heterogeneous populations
- Science of degradation and lifetime prediction
Harnessing Coherence in Light and Matter

The transformative opportunity is the potential ability to realize full control of large-scale quantum-coherent systems... the potential to revolutionize diverse fields through the control of the outcome of chemical reactions or the instantaneous state of a material.

- new real-time quantum microscopes that can visualize and control quantum matter
- Long-lived temporally coherent states of quantum wavefunction
- Ability to suppress decoherence effects of the environment
- Role of symmetry protected states in coherent matter
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.
Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales

Making and exploiting advances in imaging capabilities emerge as national priorities because of their transformative impacts on materials discovery. … accelerating the introduction of new materials, the understanding of combustion and other chemical processes, and progress in materials synthesis; and solving longstanding challenges in the relationship between the structure of inhomogeneous matter and its behavior.

- Attosecond measurements
- High resolution, chemically resolved multiscale mapping
- 4D characterization
- Advanced, spatially & temporally resolved spectroscopy
Enabling Success

From the 2007 report: “In particular, the following needs were identified:
  • A highly trained, diverse, and empowered scientific workforce...;
  • A group of theorists, concentrating on the very difficult and demanding fundamental questions...; and
  • Appropriate new experimental and computational facilities...”

BES responded, and action led to:
   EFRCs, SC Early Career Awards, SISGRs

As we look to the future,
the opportunity to accelerate progress is clear, & compelling needs remain
  • Synthesis
  • Instrumentation and Tools
  • Human Capital
**Predicting functionality**

A central element of control science is the ability to predict functionality in complex, non-equilibrium, and dynamic materials. This will require embracing computational materials science, materials genomics, and predictive inverse design.

**Making functional materials**

The science of synthesis includes not only knowing what one wants to make but also knowing how to make it. We need to grow a synthesis capability consistent with the magnitude and sophistication of our characterization and computational resources.

*BES should lead the way in embracing computational materials science, advanced synthetic approaches, and their integration as critical initiatives to accelerate materials discovery*
• New eyes yield new insights. Advances in technology such as lasers, scanning probes, and x-ray, neutron and electron sources enable imaging of dynamic and coherent phenomena that cannot otherwise be accessed.

• This new generation of instruments should be fully linked to emerging mathematical and computational capabilities to accelerate understanding and discovery.

• Tools for coordinated multi-modal and in situ measurements are required to observe and exploit heterogeneous materials and hierarchical architectures across multiple length and time scales

**BES should enhance its commitment to investigators skilled in instrument development and technique creation in order to plant the seeds for the next generation of experimental, mathematical, and computational capabilities that will advance the frontiers of discovery science and inspire future large-scale facilities**
Human Capital & Resources

• It is critical to attract, train and sustain the next generation of innovative scientists who will develop and use disruptive methods to pursue the transformative opportunities presented in this report. Innovative and strategic programs that focus on transformative science must be continuously created, refined, and sustained. Especially in times of fiscal constraint, BES should ensure a balanced portfolio of investments.

• Networks of scientists spanning synthesis, characterization, theory and simulation are necessary for effectively meeting the grand challenges. BES should strengthen the connections and continue to foster the next generation of energy scientists who can span disciplines through collaboration.
Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science

- Instrumentation & Tools
- Human Capital
- Synthesis

- Mastering Hierarchical Architectures
- Beyond Ideal Materials and Systems
- Harnessing Coherence in Light and Matter

- Imaging Matter across Scales
- Data, Algorithms and Computing
- Energy and Information on the Nanoscale

- Efficient Synthesis for Tailored Properties
- Control at the Level of Electrons

- Correlated Systems
- Systems Away from Equilibrium
Work that still remains (i)

Respond to your feedback (pre-BESAC and now)
• The current print version is already out-of-date
  (due to your constructive and helpful feedback)
  (I found three “typos” on the plane...)
• Exec Summary & Intro need one more pass through cliché filter
• (your feedback today and tomorrow)
Work that still remains (ii)

Complete production layout
- embedded sidebars
- high-res images
- reference consistency; figure permissions

Chapter 2

THE GRAND CHALLENGE FOR QUANTUM CONTROL OF ELECTRONS IS TO CONTROL MATERIAL PROCESSES AT THE LEVEL OF ELECTRONS.

There are several approaches to achieving this goal. One approach is to develop quantum control technologies that can be used to manipulate the motion of electrons. These technologies include electronic and optical methods, as well as physical and chemical methods. Another approach is to develop new materials that can be used to create quantum control devices. These materials include quantum dots, quantum wires, and quantum wells. Finally, there are several approaches to developing new quantum control devices, including photonic devices, electronic devices, and biological devices.

Quantum Control of Electrons in Atoms, Molecules, and Materials: Creating a New Language for the Behavior of Electrons

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