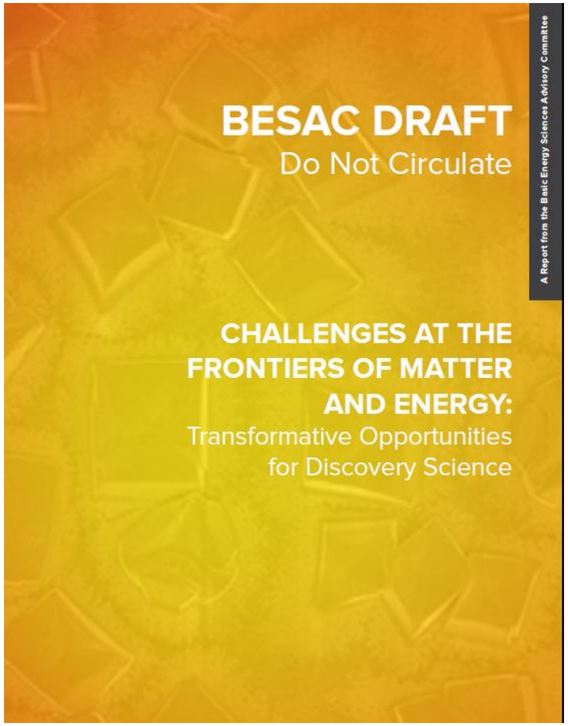
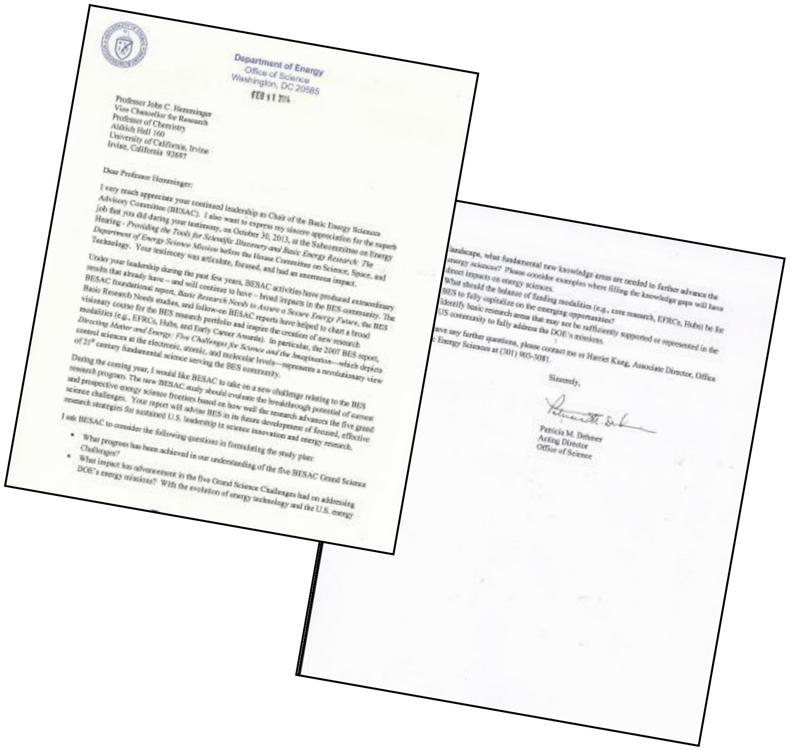
# Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science




BESAC

07/07/15

# BESAC New Charge on Strategic Planning for BES Research



Department of Energy
Office of Science
Washington, DC 20585

FEB 11 2014

Professor John C. Hemminger
Vice Chancellor for Research
Professor of Chemistry
Aldrich Hall 160
University of California, Irvine
Irvine, California 92697

Dear Professor Hemminger:

I very much appreciate your continued leadership as Chair of the Basic Energy Sciences Advisory Committee (BESAC). I also want to express my sincere appreciation for the superb job that you did during your testimony, on October 30, 2013, at the Subcommittee on Energy Hearing - *Providing the Tools for Scientific Discovery and Basic Energy Research: The Department of Energy Science Mission* before the House Committee on Science, Space, and Technology. Your testimony was articulate, focused, and had an enormous impact.

Under your leadership during the past few years, BESAC activities have produced extraordinary results that already have – and will continue to have – broad impacts in the BES community. The BESAC foundational report, *Basic Research Needs to Assure a Secure Energy Future*, the BES Basic Research Needs studies, and follow-on BESAC reports have helped to chart a broad visionary course for the BES research portfolio and inspire the creation of new research modalities (e.g., EFRCs, Hubs, and Early Career Awards). In particular, the 2007 BES report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*—which depicts control sciences at the electronic, atomic, and molecular levels—represents a revolutionary view of 21st century fundamental science serving the BES community.

During the coming year, I would like BESAC to take on a new challenge relating to the BES research program. 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 the evolution of energy technology and the 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 basic research areas that may not be sufficiently supported or represented in the US community to fully address the DOE's missions.

...ave any further questions, please contact me or Harriet Kung, Associate Director, Office ... Energy Sciences at (301) 903-3081.

Sincerely,

Patricia M. Dehmer
Acting Director
Office of Science

From: Dr. Pat Dehmer (Acting Director of Office of Science)

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# 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)**
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John Sarrao, Chair (LANL)
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
  - 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

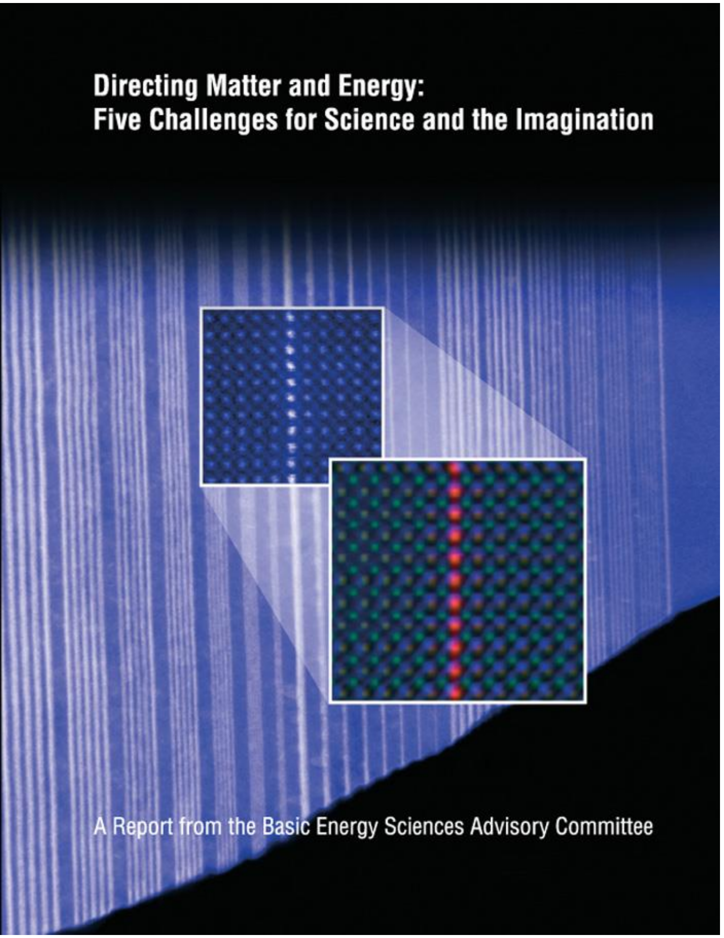
- Tuesday am (this talk): Review of the report's message and how it's captured in the printed document
- Tuesday pm: BESAC discussion/detailed feedback on open issues needing attention
- Wednesday am: Our plan of attack for responding to your feedback & sending the report to press asap

## Table of Contents

# 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”

Chapter 1

Answers to the five interconnected questions posed in the Grand Challenges report will provide fundamental knowledge to open doors to transformational technologies on several fronts, including energy, information and communication, and materials. As noted in that report, imagine a clean, affordable, and virtually unlimited supply of electrical power from solar-energy systems modeled on the photosynthetic processes utilized by green plants, and power lines that could transmit this electricity from the deserts of the Southwest to the Eastern Seaboard at nearly 100 percent efficiency. Imagine information and communications systems, based on light rather than electrons, that could predict when and where hurricanes will make landfall, along with self-repairing materials that could survive those hurricanes. Imagine synthetic materials fully compatible, and able to communicate, with biological materials.

As is befitting Grand Challenges, the quest to provide the answers that will make such technologies possible remains ongoing and formidable, a long-term venture. However, sufficient time has passed to assess the progress that has been made on all five fronts, and so the Office of Science charged a new BESAC subcommittee. This new subcommittee reviewed the scientific landscape at the time of the original report and compared it to the landscape today. The results are presented in this report, titled “Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science.”

Just as the title of the original Grand Challenges report reflected the underlying concept of directing (controlling) matter and energy from the perspective of the Office of Basic Energy Sciences (BES) research portfolio, the title of this report reflects the breakthrough potential of current and prospective BES research, based on the advances achieved to date in answering the five Grand Challenge questions. The advances made in addressing those five original questions can now serve as a springboard to realizing five new opportunities that have the potential to transform many of today’s energy-related technologies. These five Transformative Opportunities have been identified as follows:

- 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
- Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing
- Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales

Each of these five Transformative Opportunities is described in detail in an individual chapter of this report. Each chapter presents a brief overview of the opportunity, a detailed look at some of the scientific breakthroughs that will be required to capitalize on the opportunity, and the outlook for achieving the opportunity. In addition, the report provides a chapter titled **Enabling Success** that describes the resources—both people and tools—required to realize these five Transformative Opportunities. Also in the report is an appendix titled **Grand Challenges: Then and Now** that provides a status report on the five questions in the original report and the answers that have yet to be fully revealed.

The chapter titled **Mastering Hierarchical Architectures and Beyond-Equilibrium Matter** focuses on the opportunity to provide targeted functionality in materials by controlling the synthesis of beyond-equilibrium matter and its assembly into hierarchical architectures. Matter is in

**How do we control material processes at the level of electrons?**

**Chemistry can be seen as a sort of molecular melting pot in which different types of atoms swap or share electrons. As these electronic exchanges are at the heart of material properties and chemical processes, controlling the outcome of such exchanges presents an enormous opportunity for a wide range of technologies. We have evidence of this potential in the rapid advances that have been realized in areas where we have a strong foundation of theoretical concepts and experimental probes, such as crystalline solids, polymers, and certain small molecules. With sufficient control of materials properties and chemical processes at the electronic level, it should be possible for us to mimic or even improve upon the remarkable functionality we see in biological materials, with the single-layer, soft, amorphous, and heterogeneous materials we design and make for ourselves.**

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

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How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?

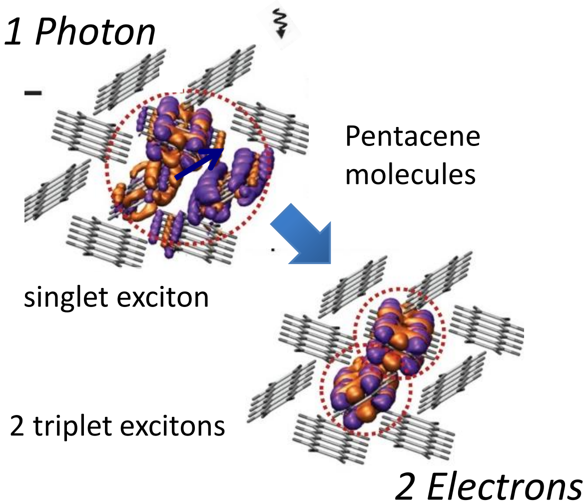
How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?

How do we characterize and control matter away - especially very far away - from equilibrium?

Advances in data, algorithms & computing, and imaging across scales will, with strategic investments, further accelerate future progress

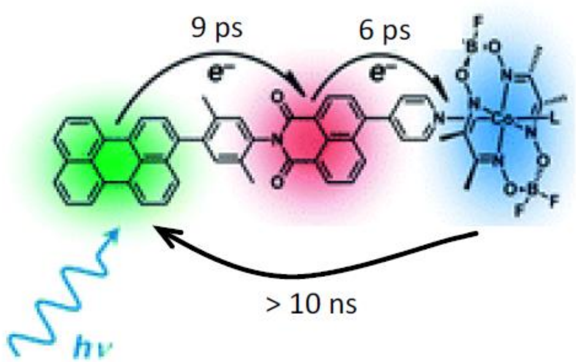
# How Do We Control Material Processes at the Level of Electrons?

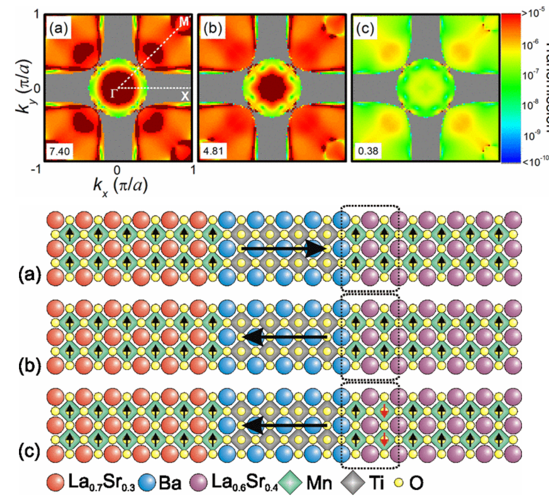
Much of the last century has focused on understanding how electrons in matter – their charge, their spin, and their dynamics – determine the properties of materials and how they direct chemical, electrical, or physical processes in materials. We are now on the verge of a new science of quantum control 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.




*Exciton Fission*

*Ultrafast Multi-step Catalysis*



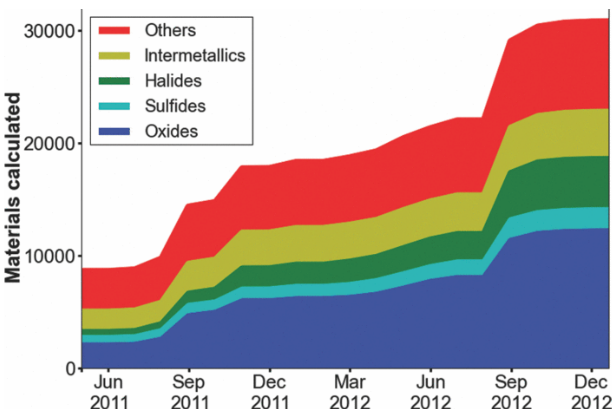

*Multiferroic Spin Valves*

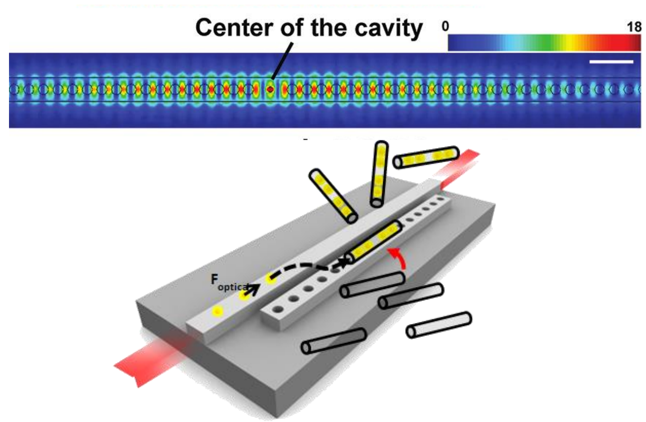
Controlling materials processes at the level of electrons has an enormously wide horizon. The broader challenges in single layer, soft, amorphous and heterogeneous materials that enable the remarkable functionality of biology and promise to bring similar complexity and functionality to artificial energy materials remain to be explored.

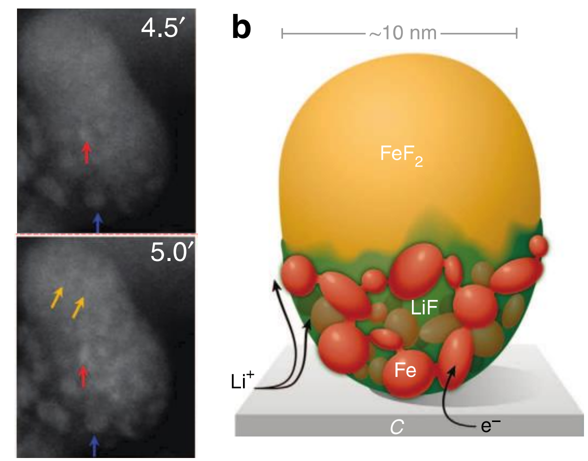
# How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?

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*

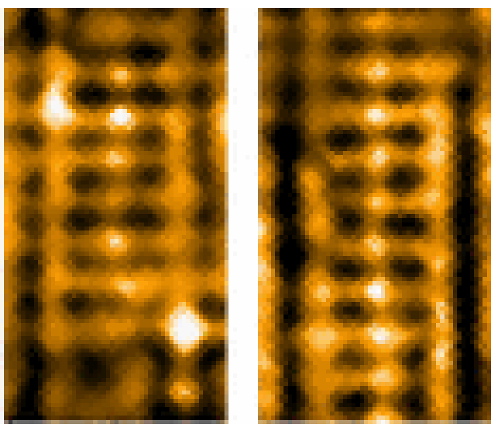
*In situ characterization*

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?

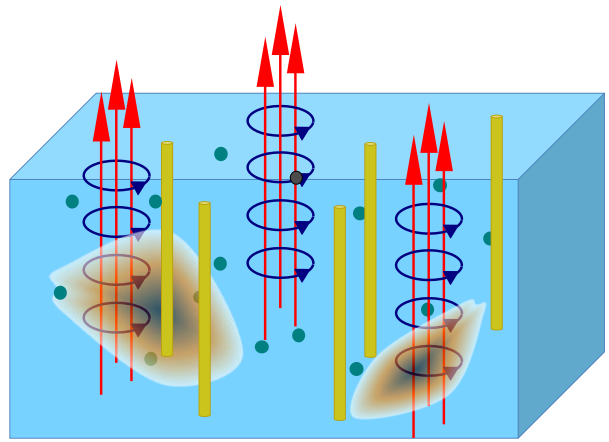
Emergent phenomena, in which the correlated behavior of many atomic or electronic constituents leads to an unexpected collective outcome, are of great significance across the sciences and engineering. Uncovering the fundamental rules of correlations and emergence is the first part of the challenge. The 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.

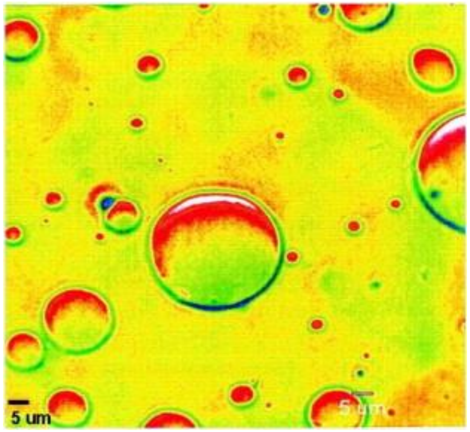
$Bi_2Sr_2CaCu_2O_{8+x}$ $Ca_{2-x}Na_xCuO_2Cl_2$



*Electronic Liquid Crystals*

*Predictive Vortex Simulation*



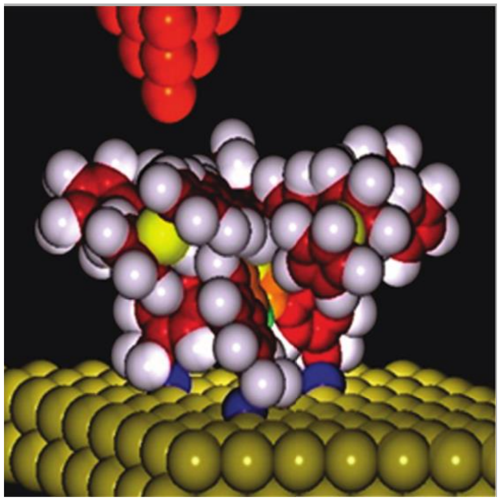



*Charged Polymers*

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.

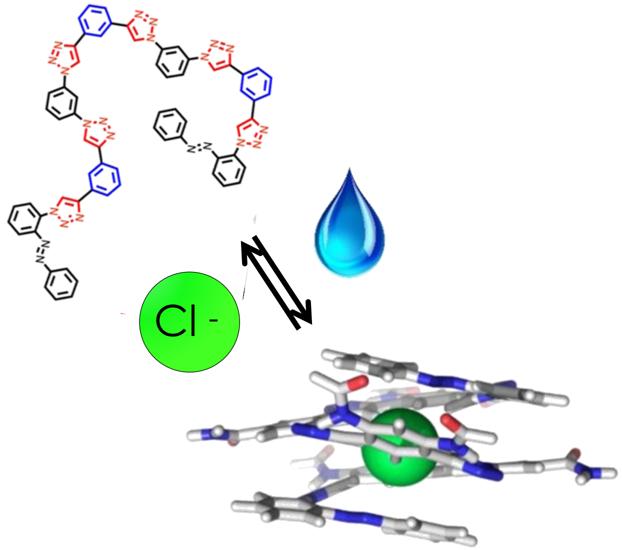
# How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?

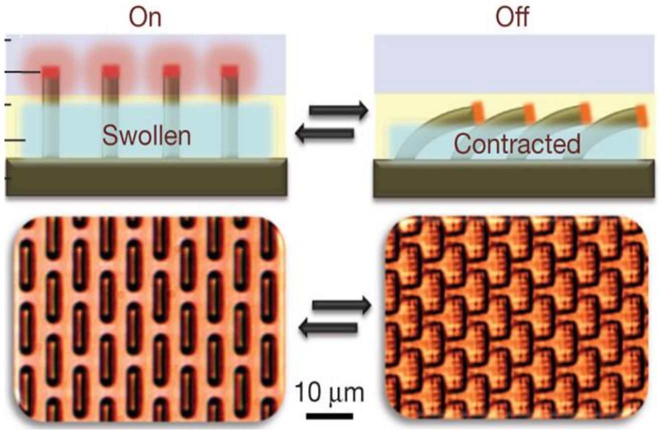
Implementation and utilization of complex nanotechnologies with capabilities approaching those found within the biological world remains beyond our reach at present. The ways in which energy, entropy, and information are manipulated within living nanosystems provide us with lessons on what humans must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



***Molecular Motors***

***Folding Polymers***



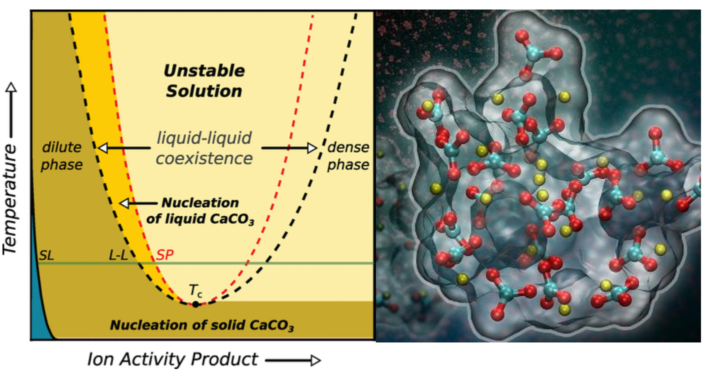




***Self-Regulation***

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.

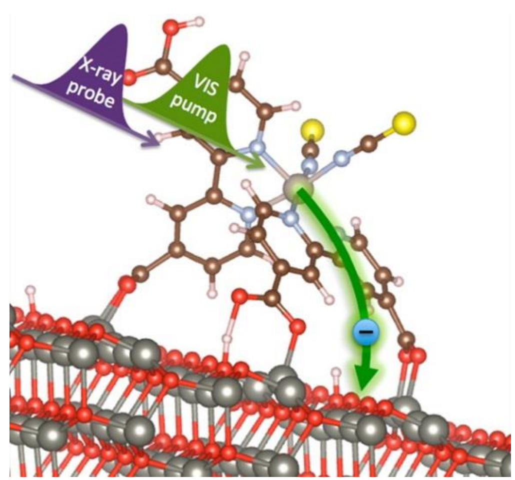
# How do we characterize and control matter away - especially very far away - from equilibrium?

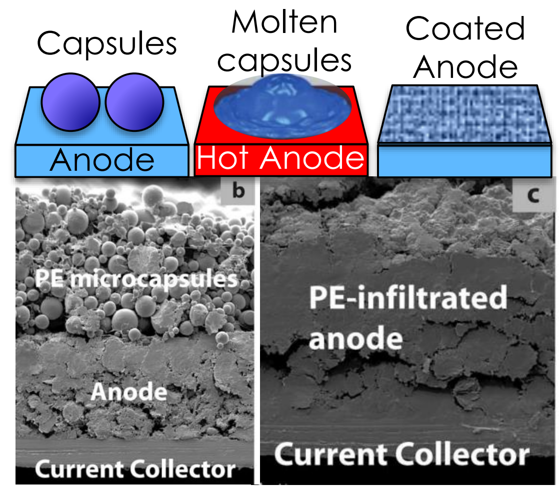
At equilibrium, we can make many significant statements about what can happen, about the states of matter and of energy, and about the structures that occur. The same is not true when we consider systems out of equilibrium, a state in which much of Nature finds itself much of the time. Understanding 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.




*Unconventional Precipitation*

*Charge Transfer Dynamics*




*Arresting Thermal Runaway*

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?

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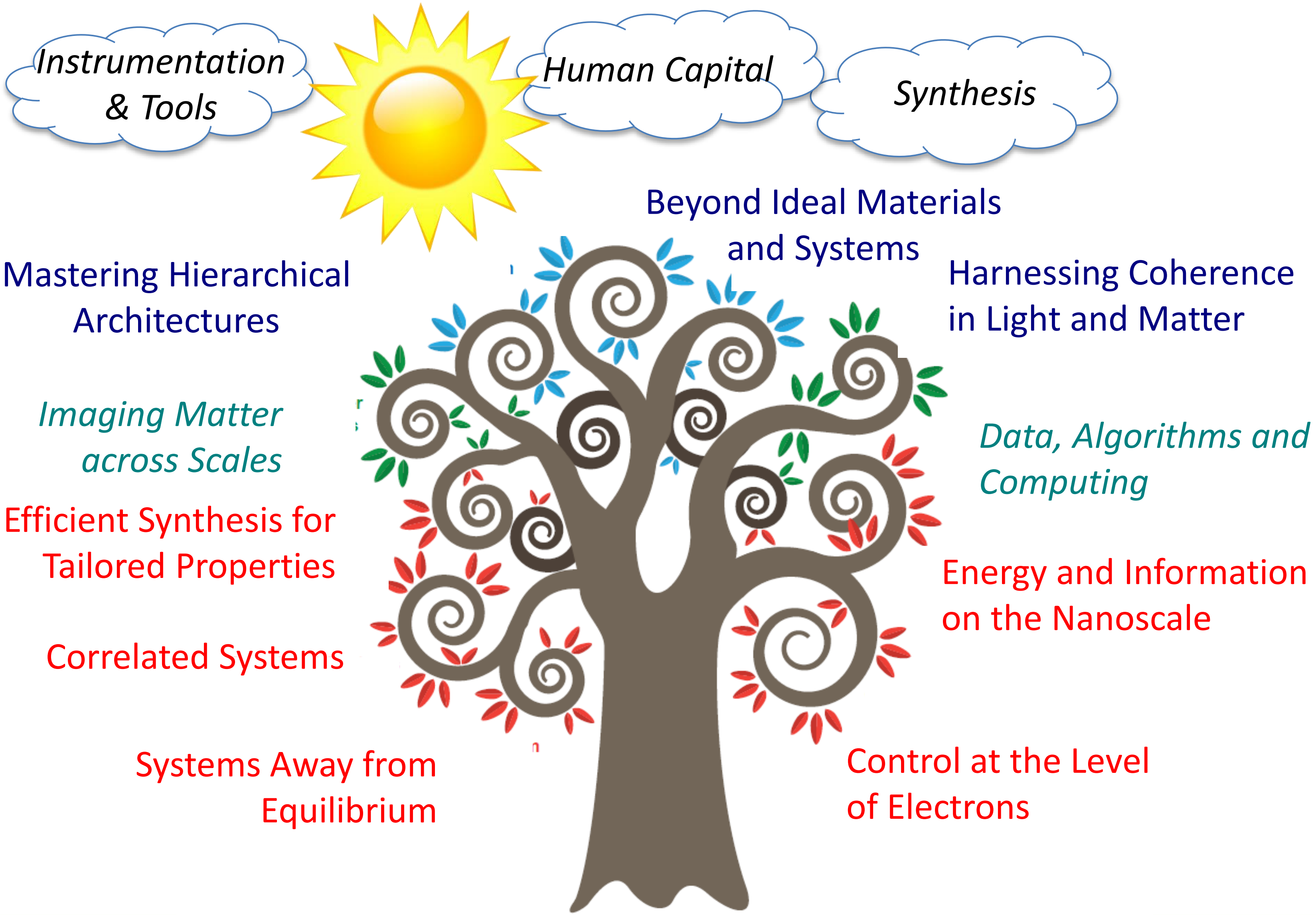


# New Transformative Opportunities have emerged that have their foundations in the Grand Challenges

*"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***

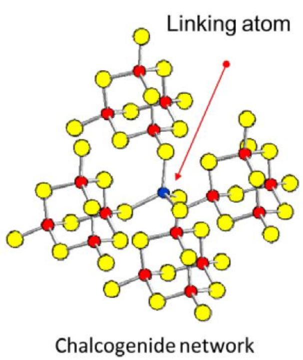
**Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing**

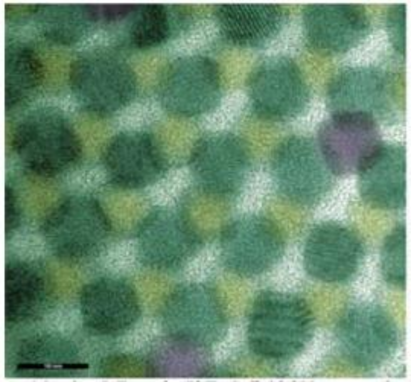
**Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales**

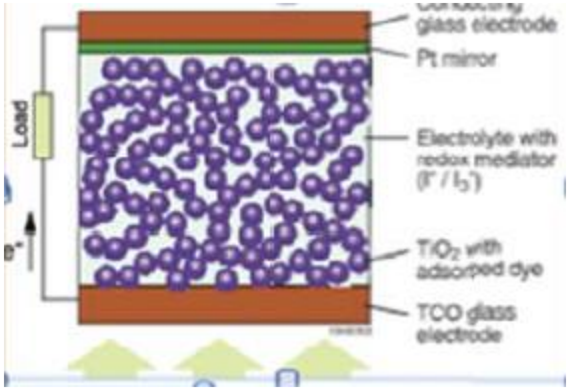
# Mastering Hierarchical Architectures and Beyond-Equilibrium Matter

*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) *in situ* characterization of spatial and temporal evolution during their synthesis and assembly



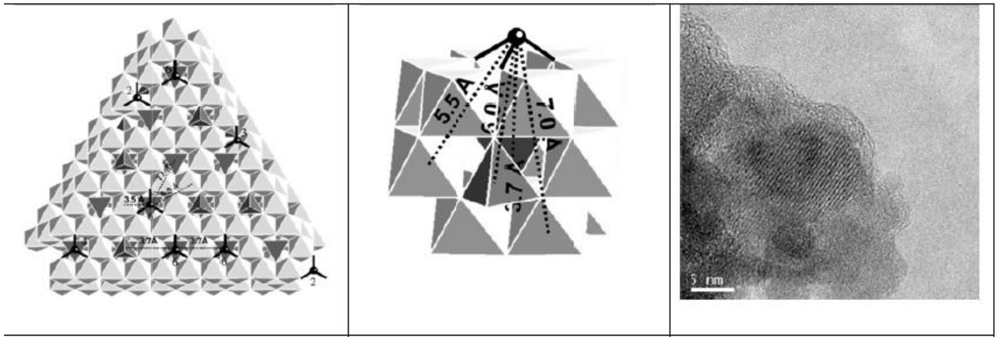


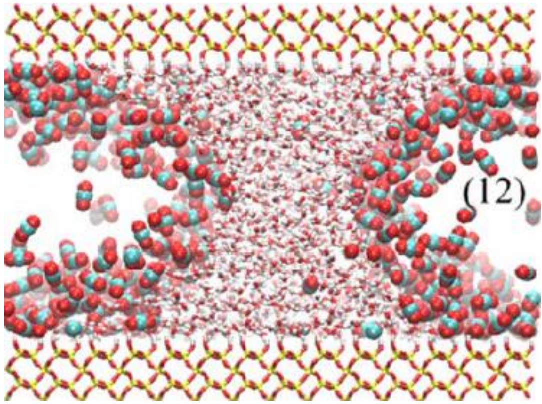
# Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces and Disorder

*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


Figure 1: Enhanced structural disorder leads to smaller overall disorder in the system (schematically).

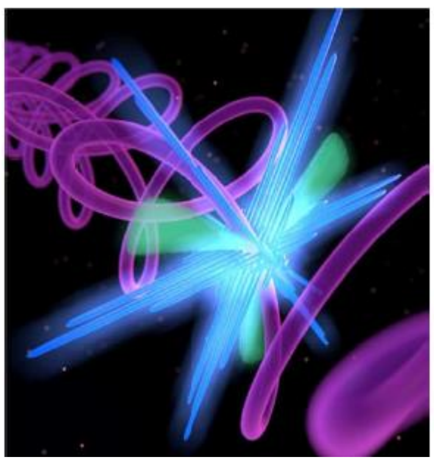


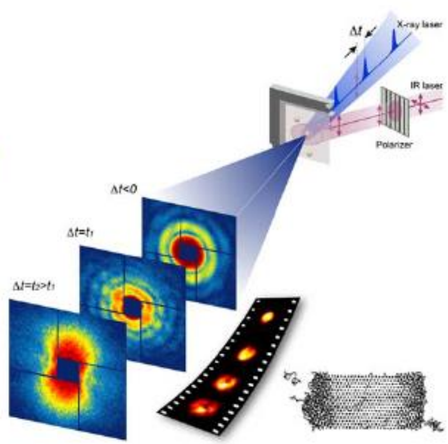


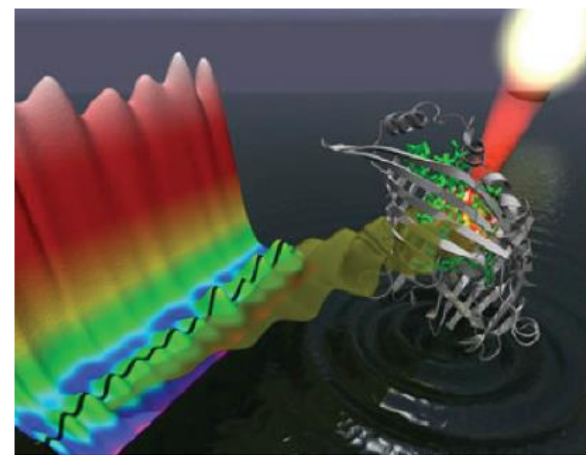
# Harnessing Coherence in Light and Matter

*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

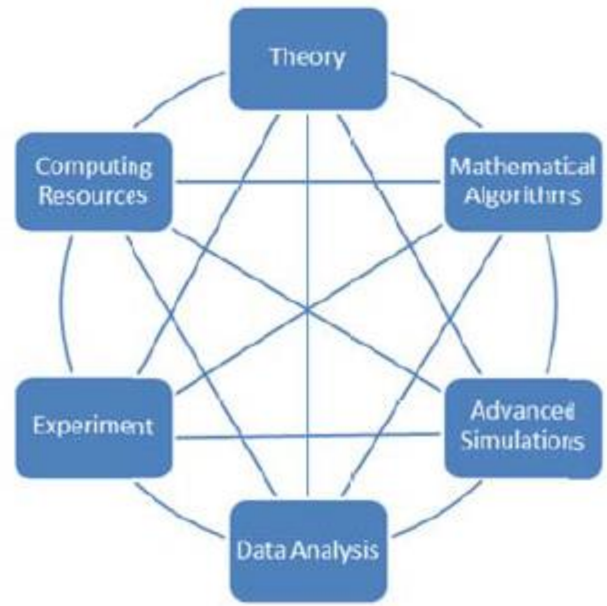


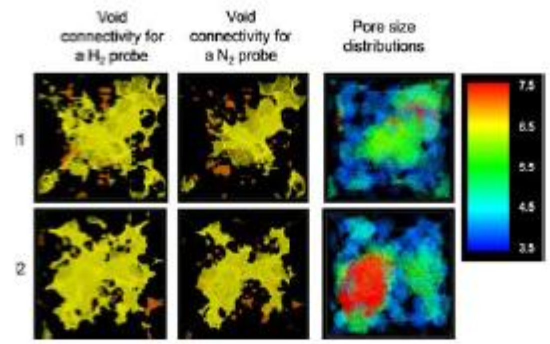


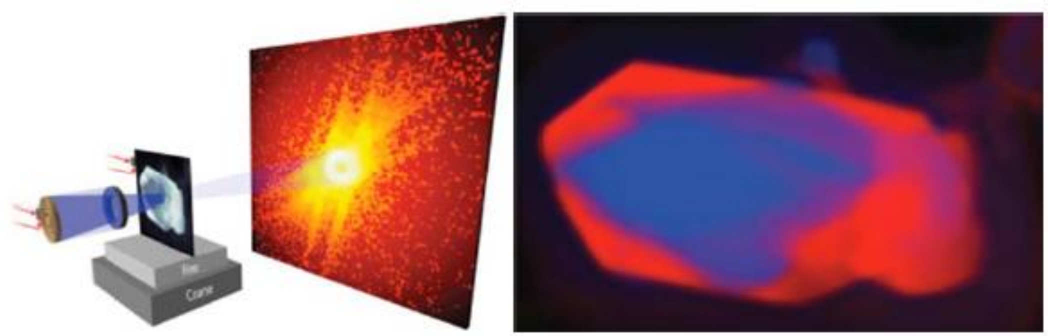



# Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing

*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.*

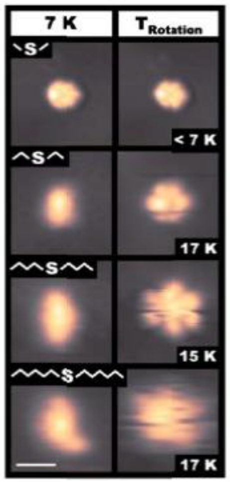


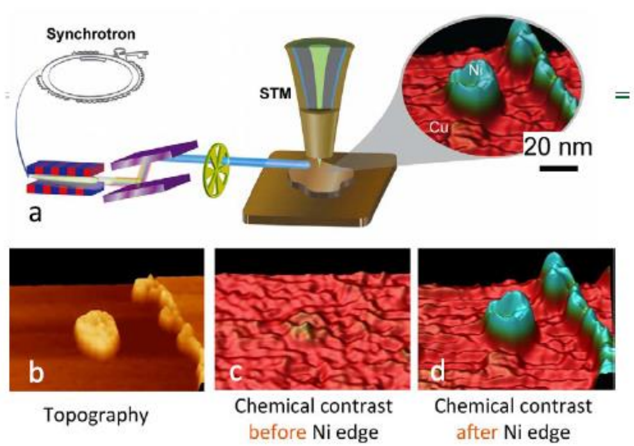



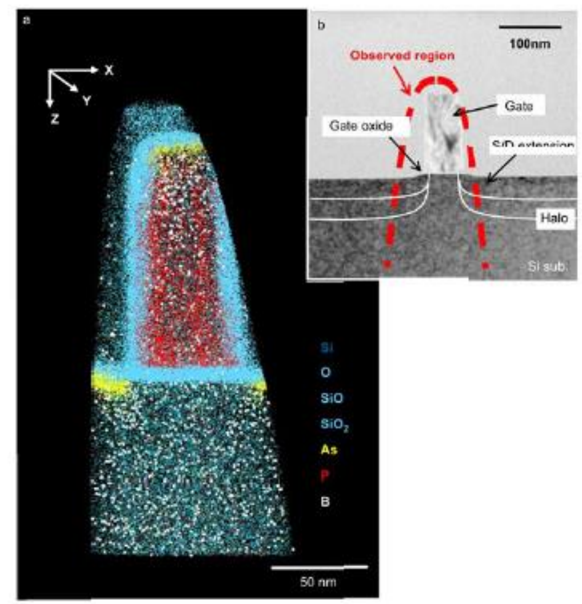



# Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales

*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

# Synthesis

### *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***

# Instrumentation & Tools

- 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

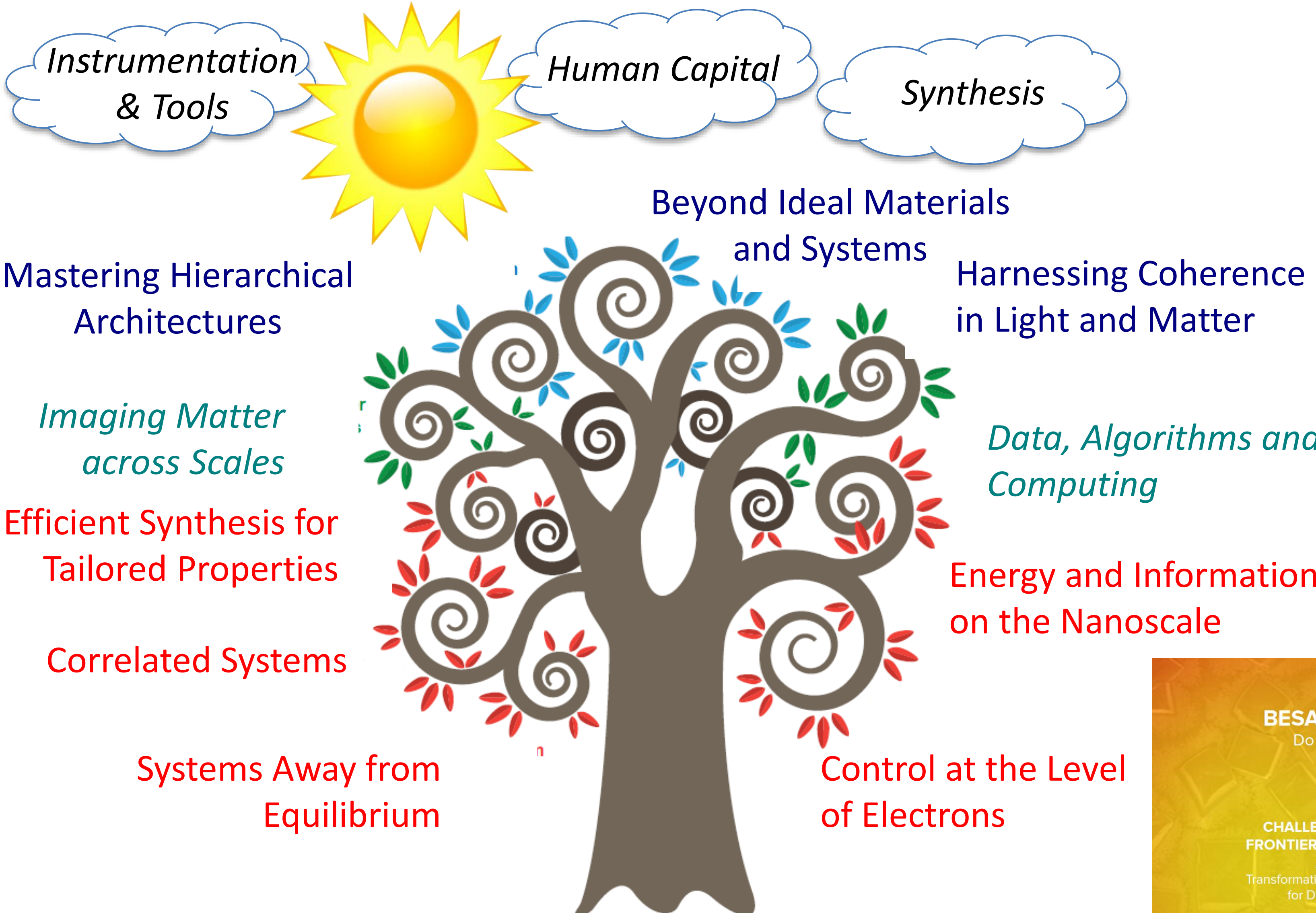
***BES should enhance its commitment to investigators skilled in instrument development and technique creation in order to plant the seeds for the next generation of experimental, mathematical, and computational capabilities that will advance the frontiers of discovery science and inspire future large-scale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

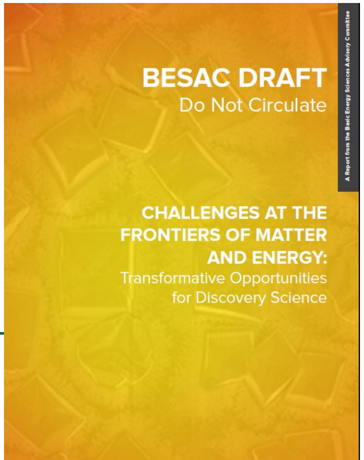
# Human Capital & Resources

- 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



# 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

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

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

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**MATERIALS, THEIR COHERANCE-BASED PROPERTIES, AND HOW WE MAY CONTROL THESE PROPERTIES IN THE FUTURE**

**Motivation and Connections to Materials**

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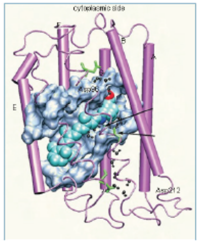


FIGURE 2.1. The retinal molecule (light blue) in the center of rhodopsin initiates a complex series of event that moves protons as part of the process of vision.

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**MOLECULAR LOGIC**

**Nanoscale communication between molecules could lead to advances in compurtation and communication**

Solar-energy conversion by photosynthetic organisms is based on the intermolecular transfer of excitation energy and electrons. These same processes may be viewed as the nanoscale exchange of information between molecules, raising the possibility that the study of such fundamental phenomena could lead not only to better methods for energy production, but also to advances in computing and communication. Most technological data transmission and processing is based on binary operations carried out by transistors and other devices arranged on the planar sub-strates of silicon "chips."

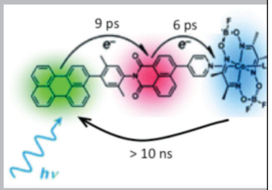


FIGURE 1. Light-controlled molecular logic gate, consisting of a porphyrin (red) flanked by two different photochromic molecules (blue), each of which can be isomerized (arrows) by light between two metastable forms.

This approach has powered the computer age, but as the search for faster, smaller, and cheaper devices continues, several problems loom on the horizon. Smaller switching devices and interconnects between them promise faster computing, but current fabrication technologies are approaching their lower limit for feature size, as discussed in Chapters 2 and 5. In addition, supercomputers now require tremendous amounts of energy. Inefficiencies in current devices contribute to this requirement, generating so much waste heat that further miniaturization of components and concurrent increases in processor capabilities are severely limited.

Some researchers are now beginning to explore information exchange between organic or bio-molecules as a prelude to molecular computing (see also Chapter 5). Many of these studies have used chemical agents to activate molecular switches, a process that occurs in the brain. Another approach that offers potential advantages is to use light as the switching agent. Light requires no wires or access for addition of chemical reagents, leads to no buildup of byproducts, and can be delivered on extremely fast time scales. Light-operated logic devices may also be rapidly reconfigured for different purposes simply by changing the nature and order of the photonic inputs.

The structure in Figure 1 is an example of a lightcontrolled molecular logic gate. By using light of different wavelengths, the molecule may be interconverted among four distinct structures. The porphyrin senses the isomeric composition of the two photochromes via elec- tron-transfer phenomena and reports on the overall structure through modulation of its fluorescence properties. This molecule may be configured by light inputs as a photonic AND Boolean logic gate, an INHIBIT gate, a 2:1 digital signal multiplexer, or a 1:2 demultiplexer.

Molecular logic devices may find application to data manipulation and storage, not as direct replacements for current technology but rather in ways we have yet to imagine.