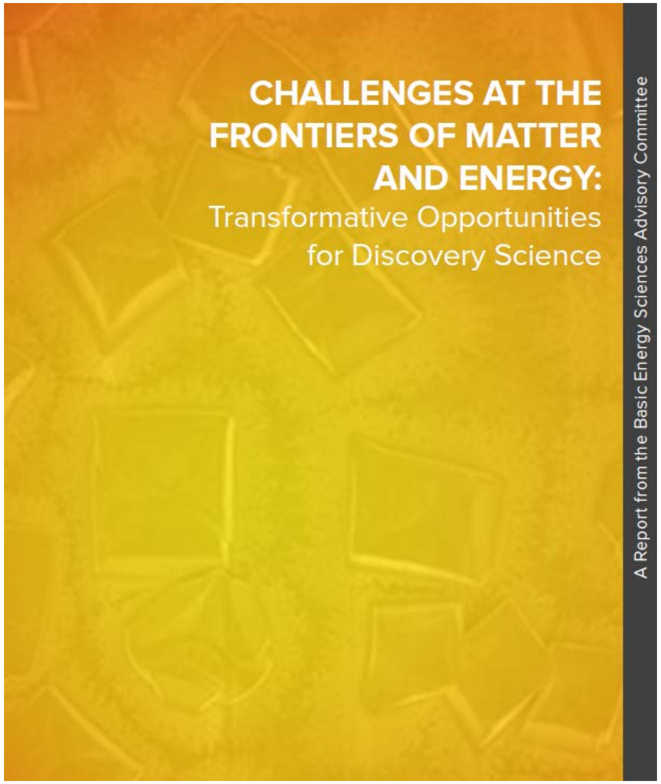
Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science



BESAC

02/11/16

John Sarrao

BESAC Subcommittee on Challenges at the Frontiers of Matter and Energy

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Lynn Yarris, Science Writer, LBNL
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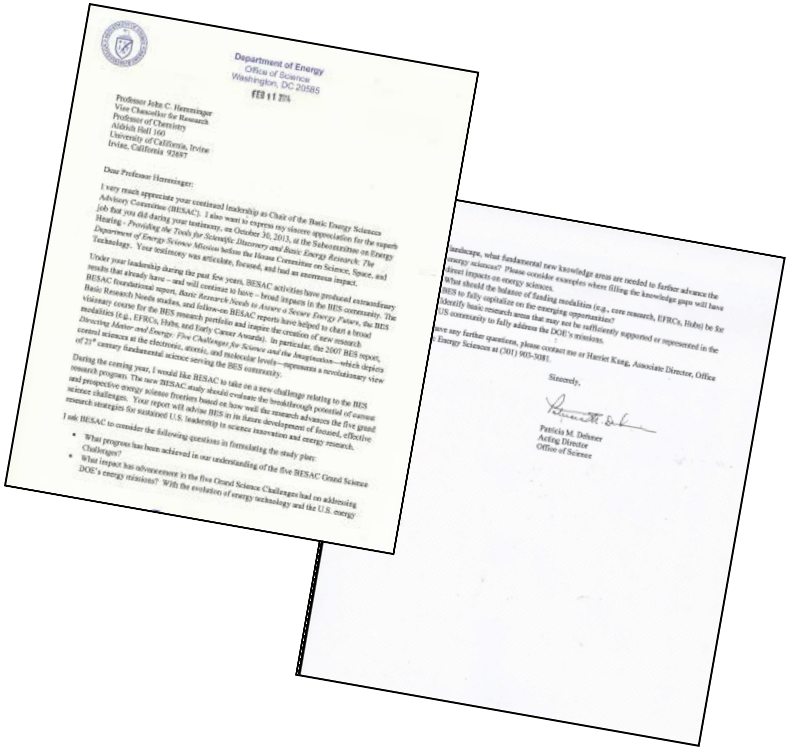
BESAC New Charge on Strategic Planning for BES Research



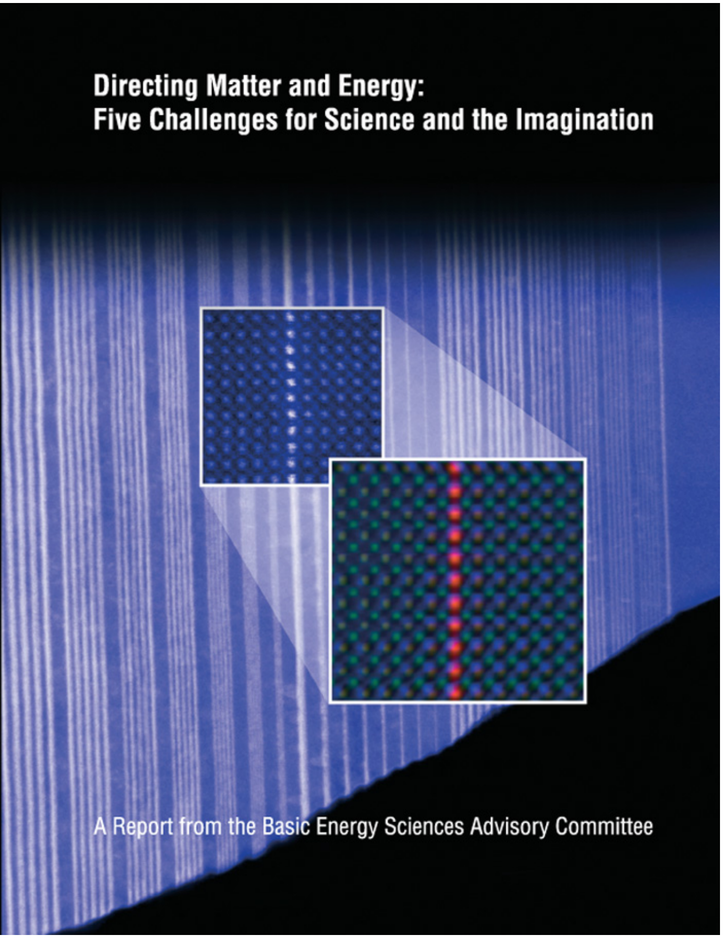
From: Dr. Pat Dehmer (Acting Director of Office of Science)

The new BESAC study should evaluate the breakthrough potential of current and prospective energy science frontiers based on how well the research advances <u>the five grand science challenges</u>. Your report will advise BES in its <u>future development of focused, effective research strategies</u> 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.

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?

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

Discovery Science Then and Now

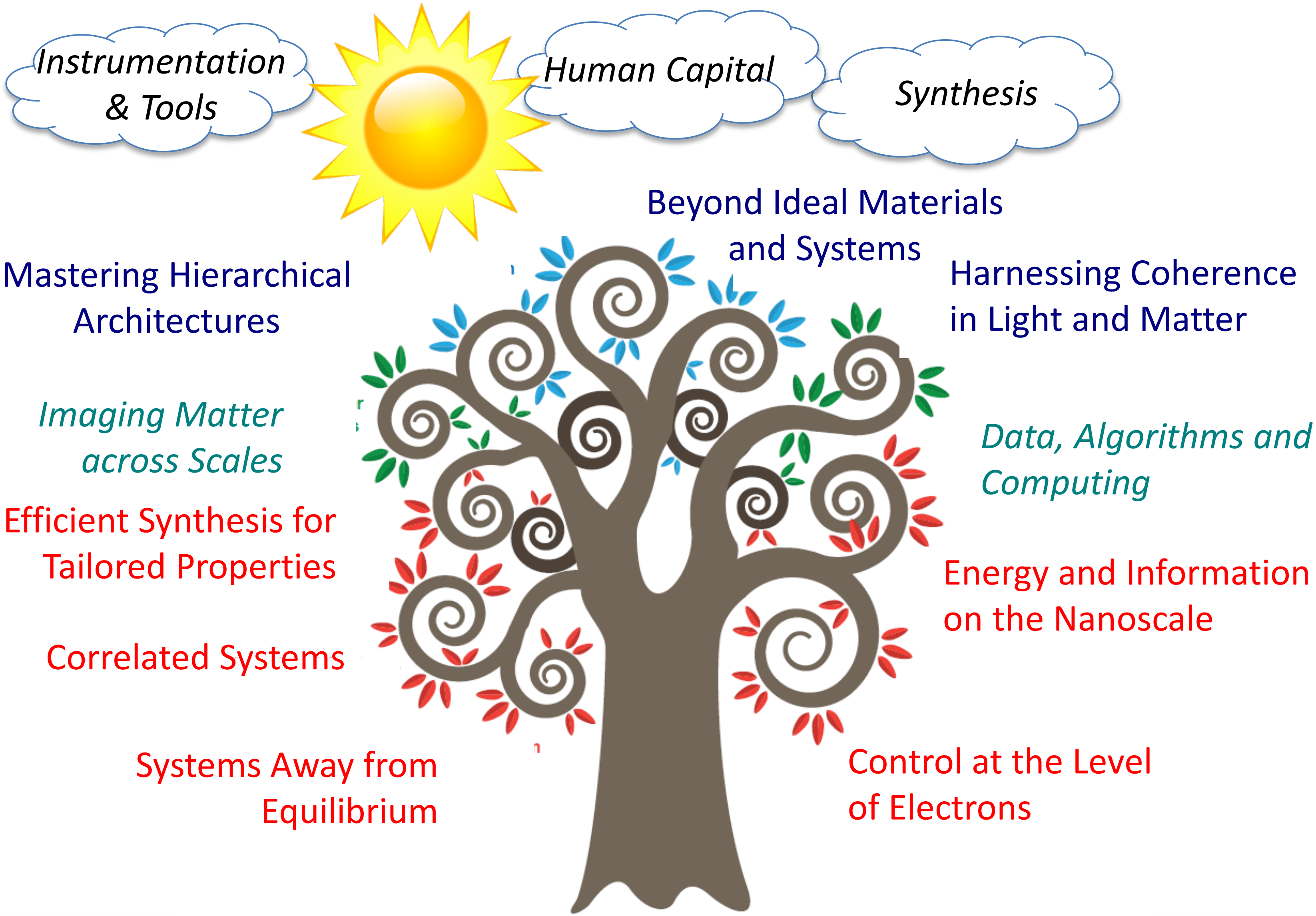
2007

- Lots of compelling research had not yet occurred
  - Graphene was rising (synthesized 2004, Nobel Prize 2010)
  - Multiferroic and magneto-electric materials (Eerenstein Nature 2006)
  - Solar cell efficiency and cost
  - 3^{rd} generation X-ray synchrotrons

2015

- 2D materials: MoS_2 and derivatives
- Symmetry, correlation and coherence: topological insulators, photosynthesis, . . .
- Organic perovskites for solar cells, . . .
- Attosecond resolution for correlated electrons with high harmonic generation lasers
- 4^{th} generation x-ray sources: LCLS coherent, ultrafast free electron laser

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



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

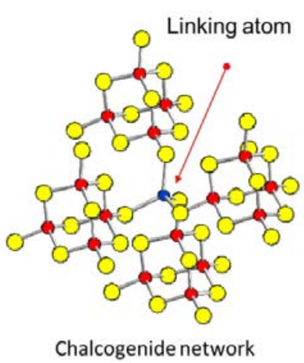
The transformative opportunity is to realize targeted functionality in materials by controlling the synthesis and assembly of hierarchical architectures and beyond-equilibrium matter, thereby increasing dramatically the exploration space for enhanced function.

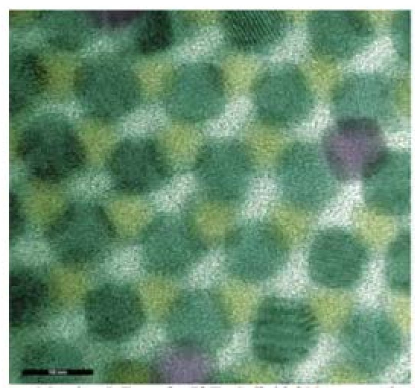
To realize this opportunity, several major advances are required:

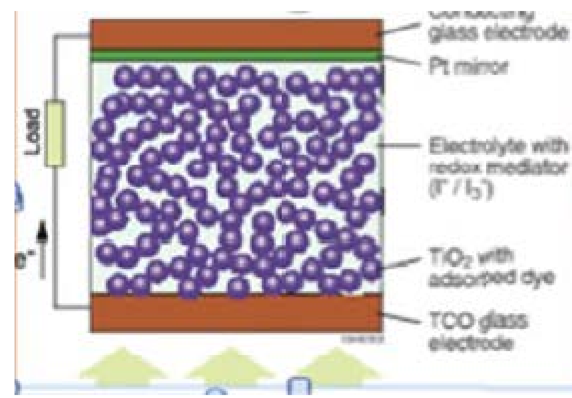
1) predictive models, including the incorporation of metastability, to guide the creation of beyond equilibrium matter

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





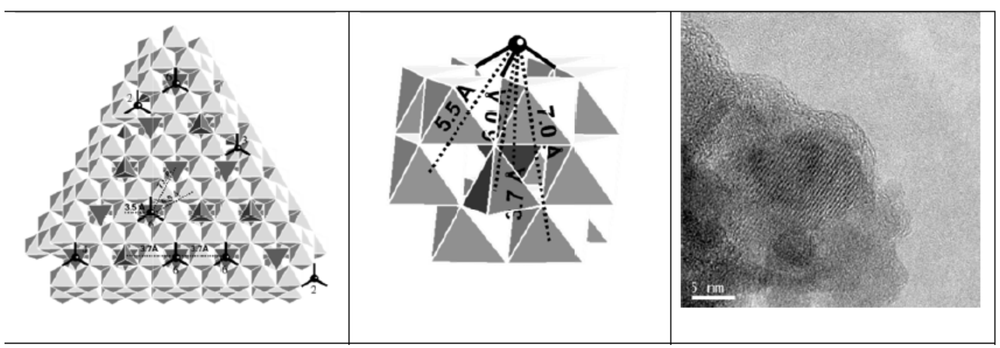


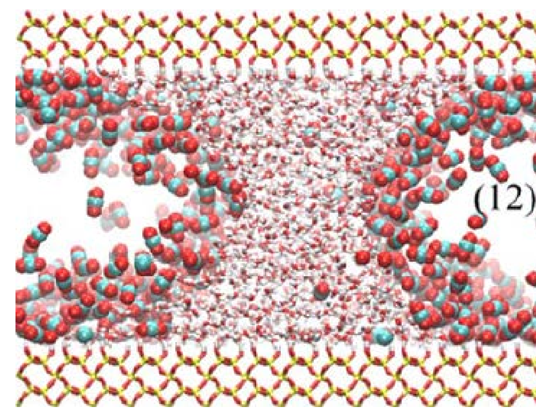
Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces and Disorder

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).

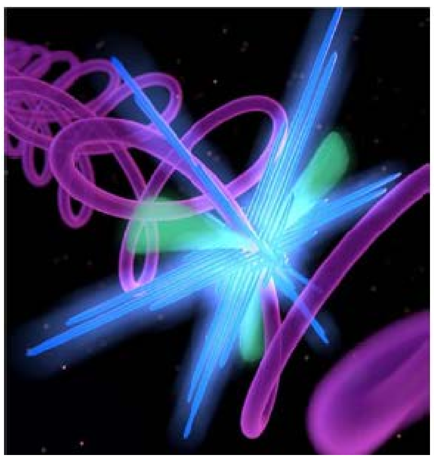


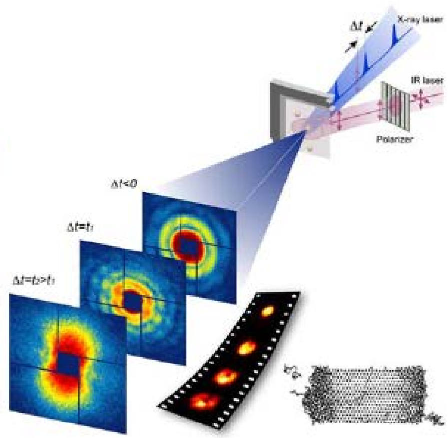


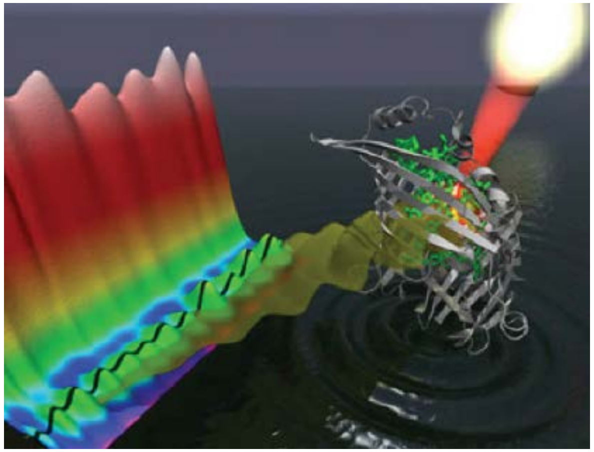
Harnessing Coherence in Light and Matter

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

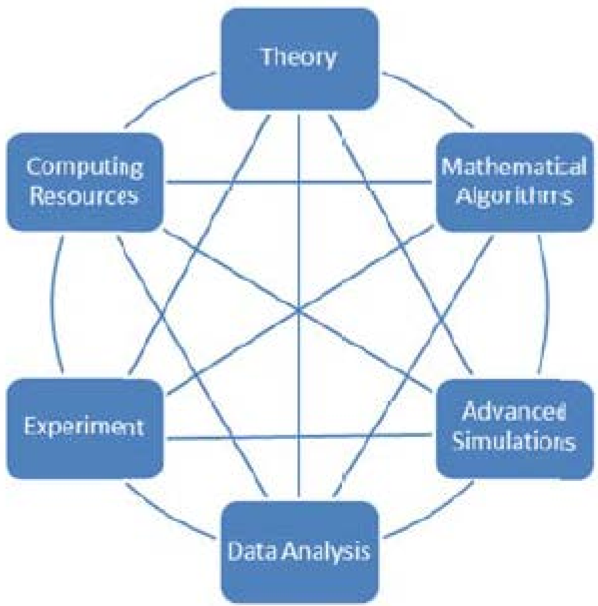


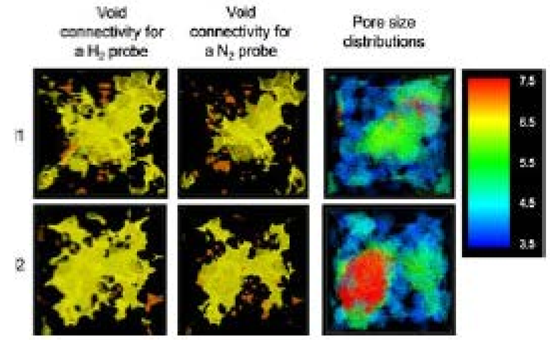


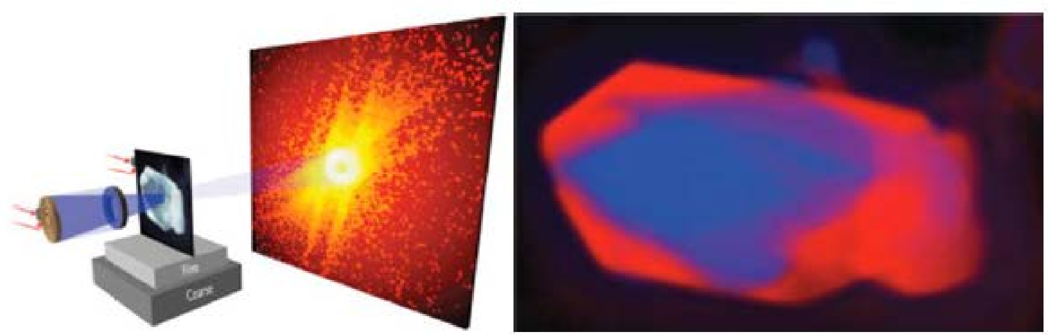


Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing

The convergence 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.

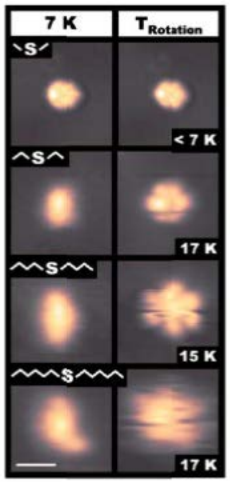


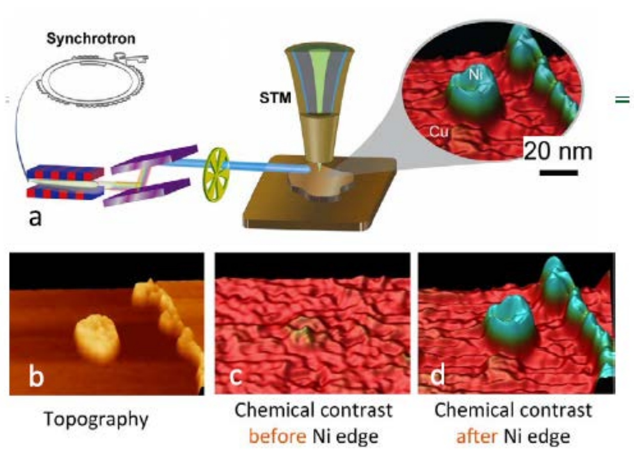


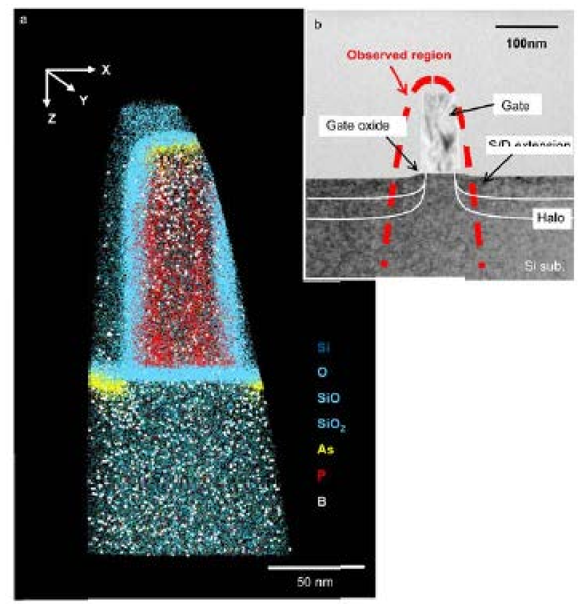


Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales

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

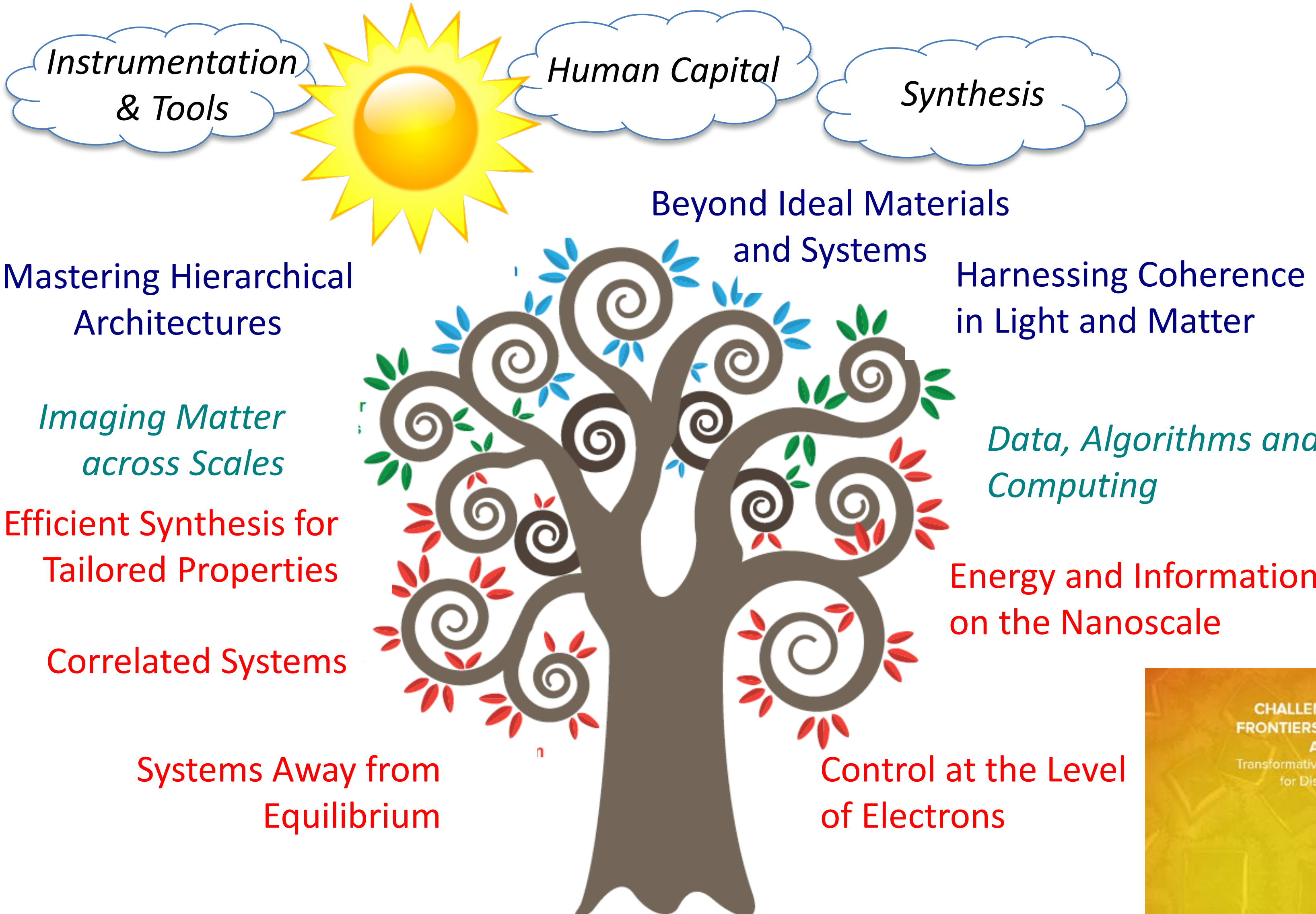
BES should enhance its commitment to investigators skilled in instrument development and technique creation in order to plant the seeds for the next generation of experimental, mathematical, and computational capabilities that will advance the frontiers of discovery science and inspire future large-scale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

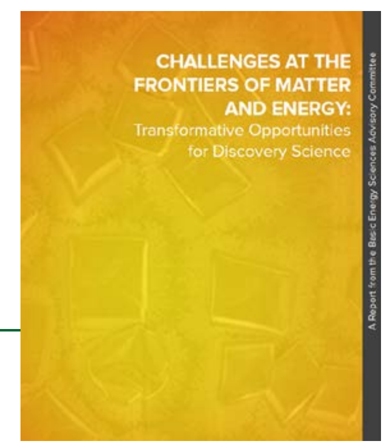
Human Capital & Resources

- 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





Basic Research Needs for Quantum Materials for Energy Relevant Technology
February 8-10, 2016

Workshop Chair: Collin Broholm (JHU)
Associate Chairs: Ian Fisher (SLAC/Stanford)
Joel Moore (UC-Berkeley/LBNL)
Margaret Murnane (UC-Boulder)
SC Technical Leads: Linda Horton and Jim Horwitz (BES)

CHARGE: Identify basic research needs and priority research directions for quantum materials with a focus on new, emerging areas with potential for transformative scientific advances and for impact on energy technologies. The phenomena of quantum materials are examined in the broad categories of: (1) superconductivity and charge-related order, (2) magnetism and spin, (3) transport and non-equilibrium dynamics, (4) electronic topology, (5) nano-structure or heterogeneity.

Breakout Sessions and Chairs:

Superconductivity and charge order: Adriana Moreo (U Tennessee) and John Tranquada (BNL)
Magnetism and spin: Meigan Aronson (Texas A&M) and Allan MacDonald (U Texas Austin)
Transport and non-equilibrium dynamics: Dimitri Basov (UCSD) and Jim Freericks (Georgetown)
Topological quantum materials: Eduardo Fradkin (U of Illinois) and Amir Yacoby (Harvard)
Heterogeneous and nano-structured quantum materials: Nitin Samarth (PSU) and Susanne Stemmer (UCSB)

Plenary Session Speakers:

- *Eli Yablonovitch, University of California-Berkeley*
- *Louis Taillefer, University of Sherbrooke (Quebec)*
- *Harold Hwang, SLAC National Accelerator Laboratory and Stanford University*
- *Alessandra Lanzara, Lawrence Berkeley National Laboratory and University of California-Berkeley*
- *Subir Sachdev, Harvard University*
- *Peter Littlewood, Argonne National Laboratory*

Basic Research Needs for Synthesis Science for Energy Relevant Technology
May 2-4, 2016

Workshop Chair: James De Yoreo (PNNL)
Associate Chairs: Robert Cava (Princeton)
Lynda Soderholm (ANL)

SC Technical Leads: Arvind Kini, Raul Miranda and George Maracas (BES)



CHARGE: Identify basic research needs and priority research directions in synthesis science with a focus on new, emerging areas with the potential to leapfrog current capabilities and impact future energy technologies.

- The workshop should identify paths to open up new frontiers to allow predictable synthesis of energy relevant materials and chemicals in a controlled manner via deterministic assembly of atoms, molecules, nanomaterials, clusters and other constituents.
- This research is essential to realize the BES Grand Challenges of “atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties” and “mastering hierarchical architectures and beyond-equilibrium matter.

Breakout Sessions and Chairs: In Progress
Plenary Session Speakers: In Progress
Background Document: “Assessment of Current Status of Synthesis Science” (In Progress)

Basic Research Needs for Innovation and Discovery of Transformative Experimental Tools — June 1-3, 2016

Workshop Chair: Ali Belkacem (LBNL)
Associate Chairs: Cynthia Friend (Harvard)
Yimei Zhu (BNL)

SC Technical Lead: Tom Settersten (BES)



CHARGE: Explore the frontiers of instrumentation science that provide opportunities to advance grand challenge energy research. The workshop will identify the scientific challenges and resulting priority research directions for instrumentation development. The workshop is expected to emphasize university-laboratory-scale instruments, portable instruments for dual use at the bench or at facility end-stations, and new concepts for experimental methods and the corresponding advanced data analytics and related approaches that are intrinsic to meaningful measurements.

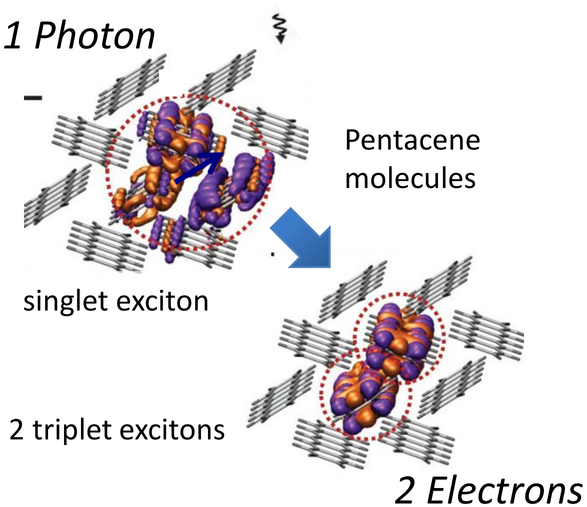
Breakout Sessions and Chairs: In Progress

- Chemical reactions and transformations in realistic environments – Beyond model systems
- Imaging materials far away from equilibrium
- Challenges of heterogeneity across multiple length scales and multiple time scales
- Transformational experimental tools through integration of instrumentation with theory and computation

Plenary Session Speakers: In Progress

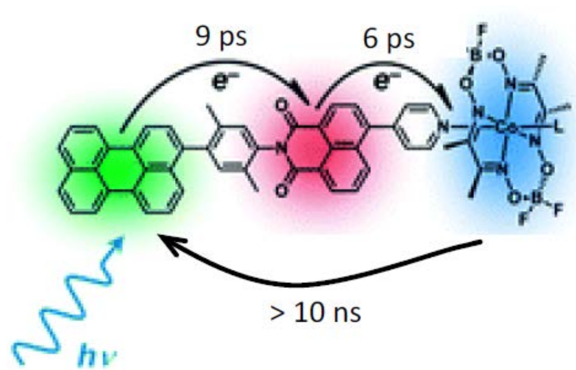
How Do We Control Material Processes at the Level of Electrons?

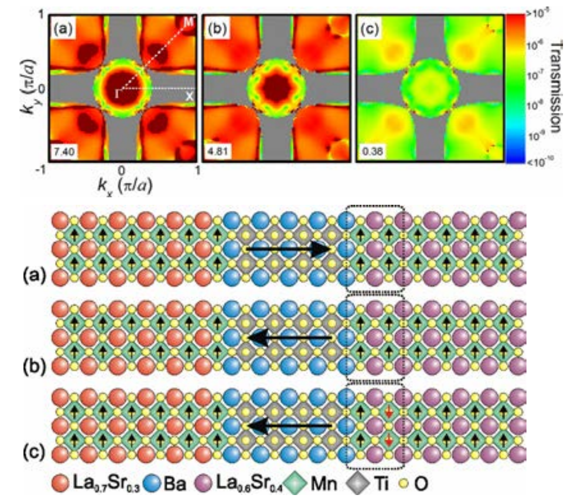
Much of the last century has focused on understanding how electrons in matter – their charge, their spin, and their dynamics – determine the properties of materials and how they direct chemical, electrical, or physical processes in materials. We are now on the verge of a new science of quantum control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





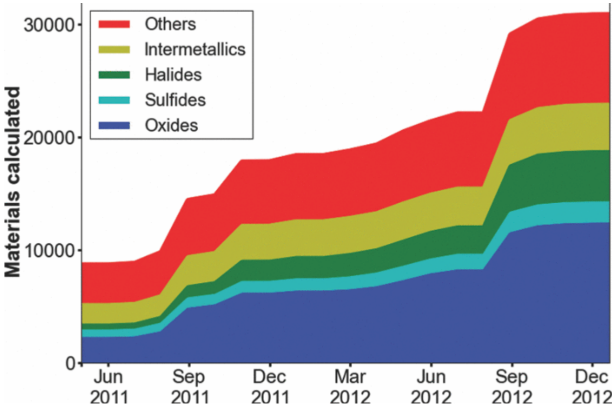
Multiferroic Spin Valves

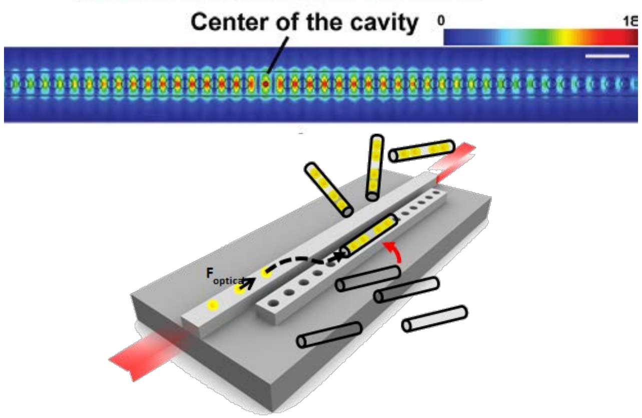
Controlling materials processes at the level of electrons has an enormously wide horizon. The broader challenges in single layer, soft, amorphous and heterogeneous materials that enable the remarkable functionality of biology and promise to bring similar complexity and functionality to artificial energy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

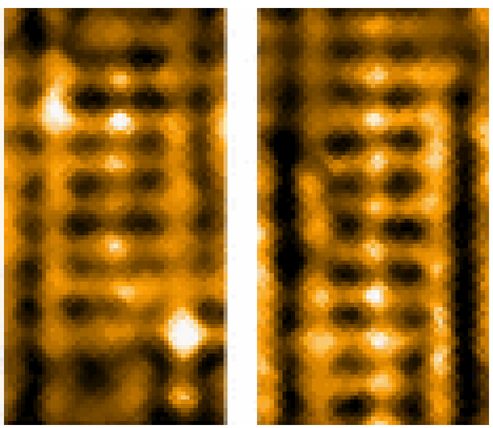
In situ characterization

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?

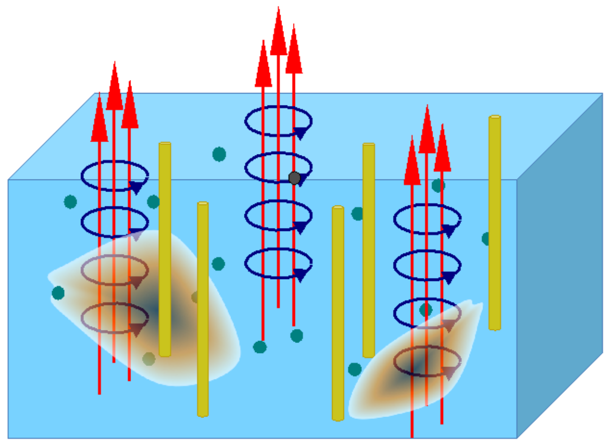
Emergent phenomena, in which the correlated behavior of many atomic or electronic constituents leads to an unexpected collective outcome, are of great significance across the sciences and engineering. Uncovering the fundamental rules of correlations and emergence is the first part of the challenge. The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

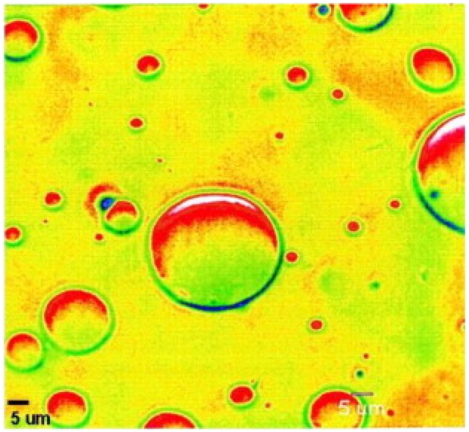
$Bi_2Sr_2CaCu_2O_{8+x}$ $Ca_{2-x}Na_xCuO_2Cl_2$



Electronic Liquid Crystals

Predictive Vortex Simulation





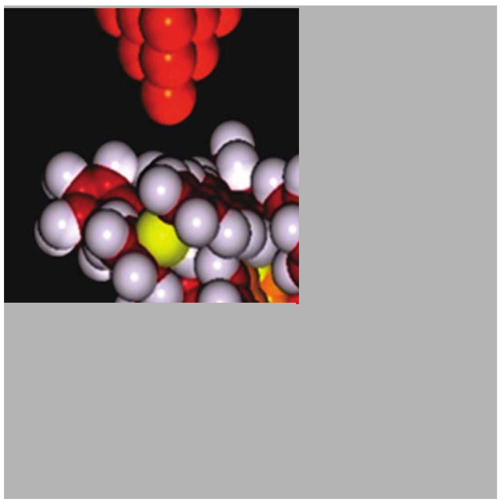
Charged Polymers

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.

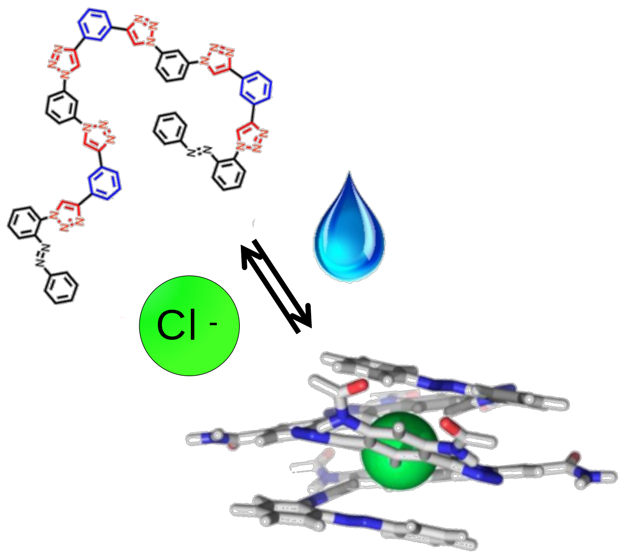
How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?

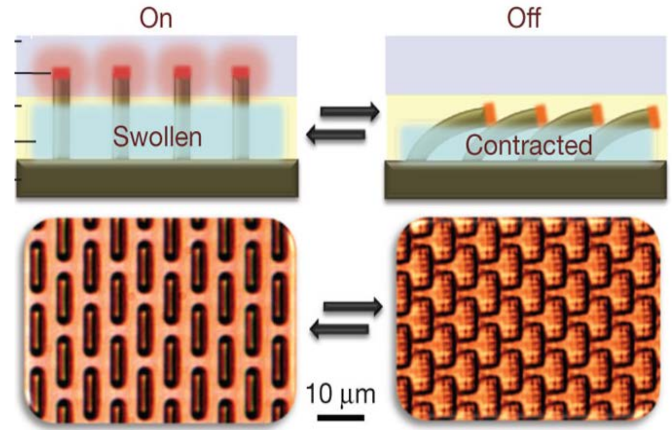
Implementation and utilization of complex nanotechnologies with capabilities approaching those found within the biological world remains beyond our reach at present. The ways in which energy, entropy, and information are manipulated within living nanosystems provide us with lessons on what humans must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

Folding Polymers



Molecular Motors



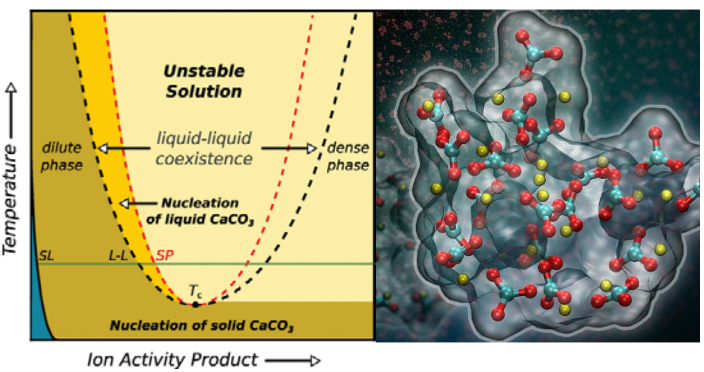


Self-Regulation

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.

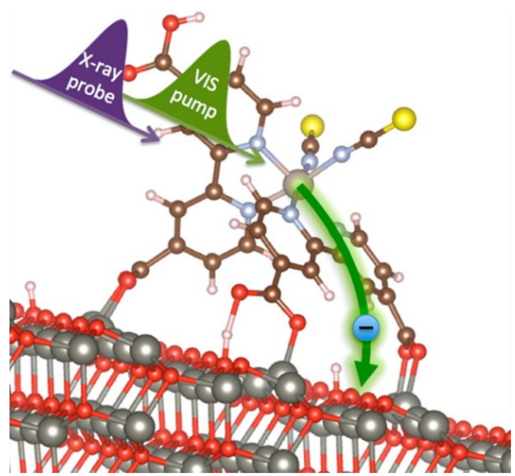
How do we characterize and control matter away - especially very far away - from equilibrium?

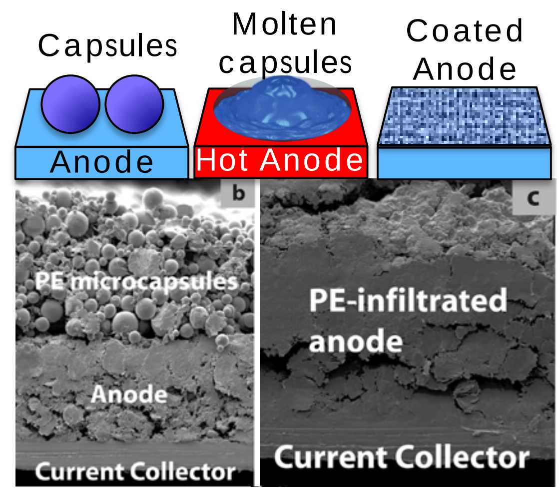
At equilibrium, we can make many significant statements about what can happen, about the states of matter and of energy, and about the structures that occur. The same is not true when we consider systems out of equilibrium, a state in which much of Nature finds itself much of the time. Understanding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



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?