# Directing Matter and Energy:
## Five Challenges for Science and the Imagination

**BESAC Grand Challenges Subcommittee**

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**23 July 2008**

# What's Been Done

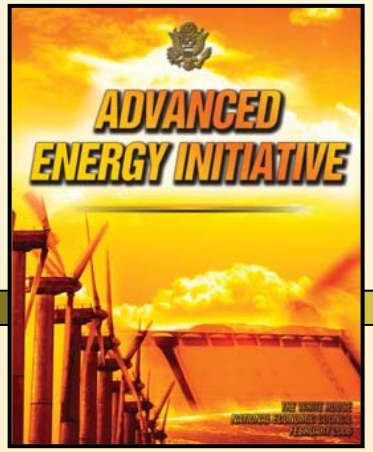
# BES and the ACI and AEI

| Grand Challenges | Discovery Research | Use-Inspired Basic Research | Applied Research | Technology Maturation & Deployment |
|---|---|---|---|---|
| ▪ Basic research to address fundamental limitations of current theories and descriptions of matter in the energy range important to everyday life – typically energies up to those required to break chemical bonds.<br>▪ Particularly challenging are the failures to understand and to contol systems that are ultrasmall or isolated, or are far from equilibrium, or display emergent phenomena of many kinds. | ▪ Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies<br>▪ Development of new tools, techniques, and facilities, including those for advanced modeling and computation | ▪ Basic research for fundamental new understanding, usually with the goal of addressing showstoppers on real-world applications in the energy technologies | ▪ Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes<br>▪ Proof of technology concepts | ▪ Scale-up research<br>▪ At-scale demonstration<br>▪ Cost reduction<br>▪ Prototyping<br>▪ Manufacturing R&D<br>▪ Deployment support |

BESAC & BES Basic Research Needs Workshops

DOE Technology Office/Industry Roadmaps

BESAC Grand Challenges Panel



# Why now?

- **Necessity**
  - Natural resources declining
  - Advanced technologies adversely affecting environment
  - Science and technology keys to better tomorrow
- **Opportunity**
  - <u>Sustainable</u> advancement
  - Newfound ability to probe and understand microscopic quantum world
  - Control matter and energy at the quantum level

# A Grand Challenge Must…

- Be scientifically deep and demanding
- Be clear and well-defined
- Be relevant to the broad portfolio of BES
- Promise real dividends in devices or methods that can significantly improve the quality of life and secure the energy future for the United States

# Grand Challenges—Process

**We collected suggestions for grand challenge questions from members of BESAC & the Grand Challenge subcommittee. Some of the many examples:**

Can we create complex functional materials that can be fully disassembled and re-assembled?

Can we design and build self-regulating, self-repairing molecular devices?

Actively enhancing our predictive understanding of strongly-correlated electronic materials.

Can we build devices that fully integrate living and nonliving components?

The dynamics of interacting finite mass nuclei and electrons, far outside the Born-Oppenheimer approximation caused by high energy and high frequency incident radiation and particles.

# Grand Challenges—Process

Can we go the last micron? In other words, can we wire up the biological world for energy and information transfer?

Can we control transition states in chemical reactions/phase transitions to create novel compounds/materials?

What is the state of matter between solid and plasma? Can we understand high energy density matter?

Can the atomic structure of proteins be solved rapidly without need for crystallization ?

Can movies be made of molecular reactions ?

Can we design and execute reactions at solid surfaces with the same predictability and control of molecular reactions in solution?

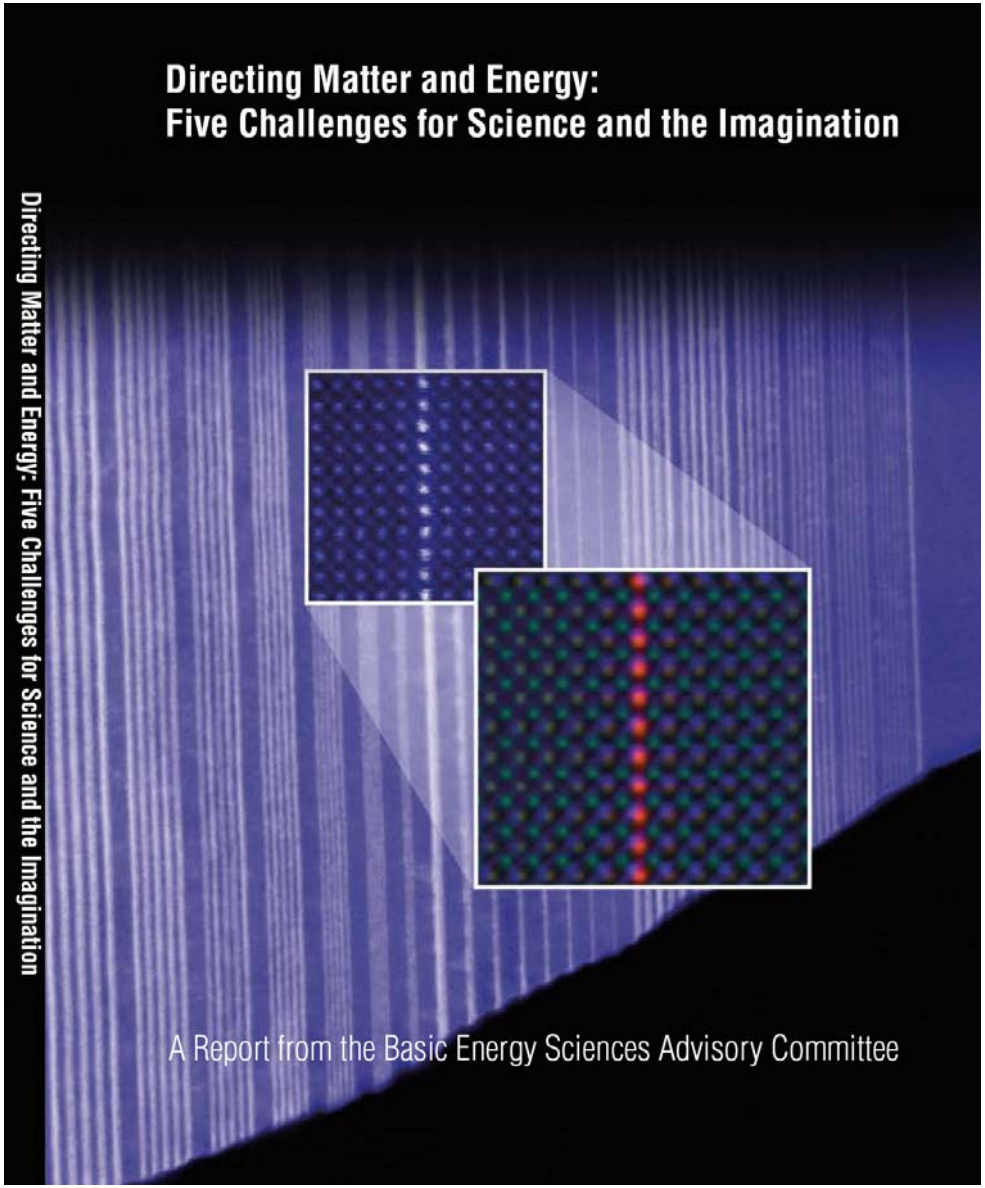
# Recurring Themes …

- We go to the very small
- We go *far* from equilibrium
- We encounter strongly correlated systems and systems with emergent properties
- We want to define the limits of material properties
- We want to manipulate energy and information ever more rapidly and efficiently
- We want to recreate in synthetic systems properties and capabilities we find in nature

# Connecting Themes:
# An Underlying Set of Concepts Emerged

**We are on the <u>threshold of a transition from observation science to control science</u> at a much deeper level than is currently possible. This idea led to five grand challenges.**

# The Report


Directing Matter and Energy: Five Challenges for Science and the Imagination
Directing Matter and Energy:
Five Challenges for Science and the Imagination
A Report from the Basic Energy Sciences Advisory Committee

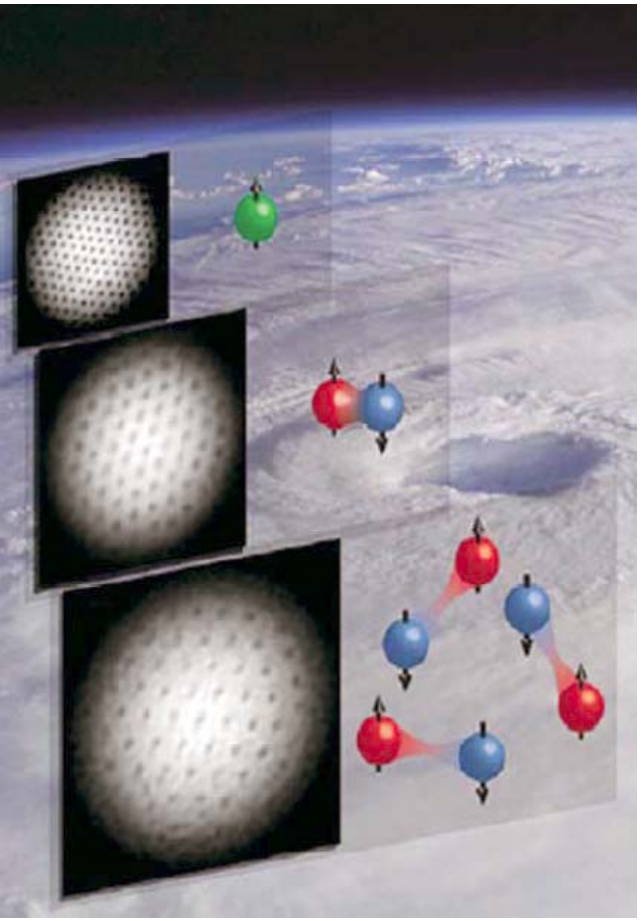
# Five Grand Challenges

1. How do we control materials and processes at the level of electrons?
2. How do we design and perfect atom- and energy-efficient synthesis of new forms of matter with tailored properties?
3. How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties?
4. Can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems?
5. How do we characterize and control matter away—especially very far away—from equilibrium?

# 1. Control material processes at the level of electrons

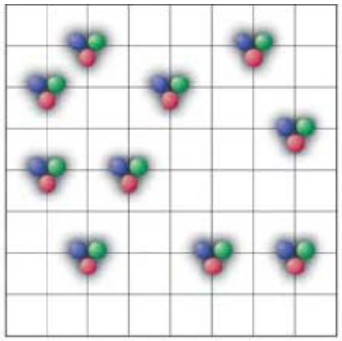
## Making quantum systems work for us—and for a desired outcome

**Microscopic vortices in atomic gases**

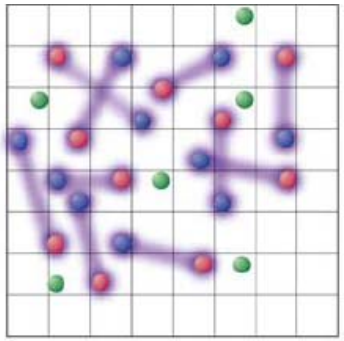


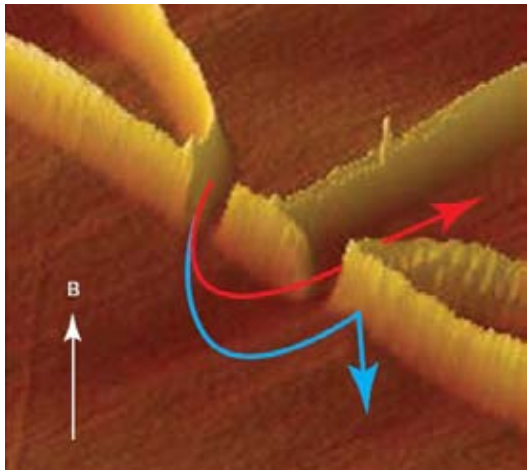
- Attosecond optical pulses, high intensity excitation need to probe strong quantum correlations
- Control of spins (spintronic devices)
- Quantum computing and the use of coherence in devices
- Quantum control in nature (light harvesting in photosynthesis, catalysis)
- Quantum simulators of nuclear matter

**3 spin-1/2 atoms**



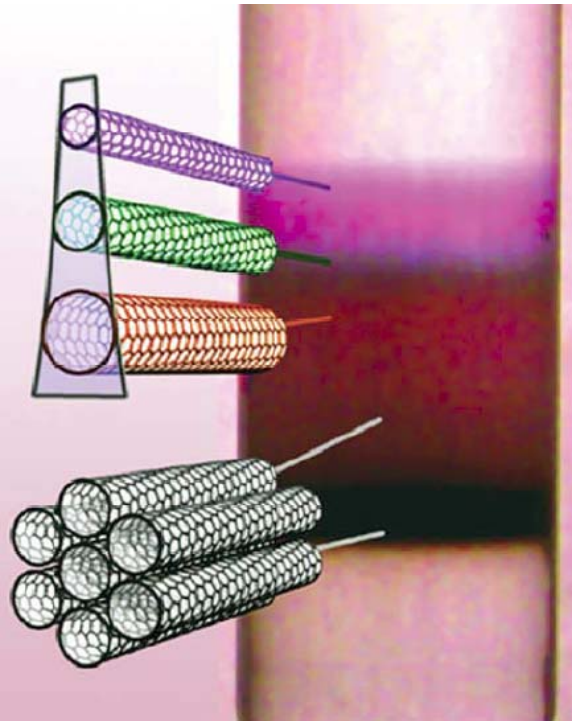
**Cooper "pairs"**



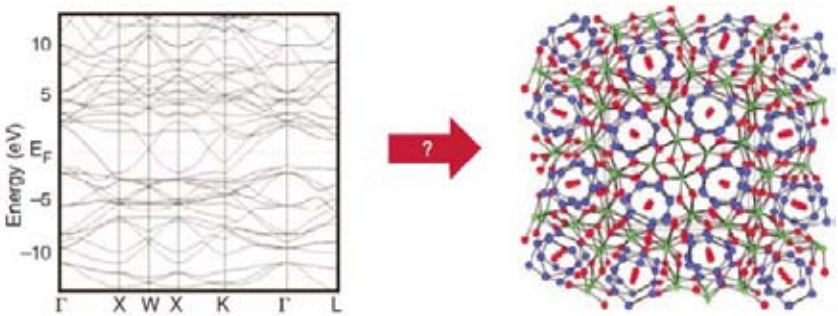


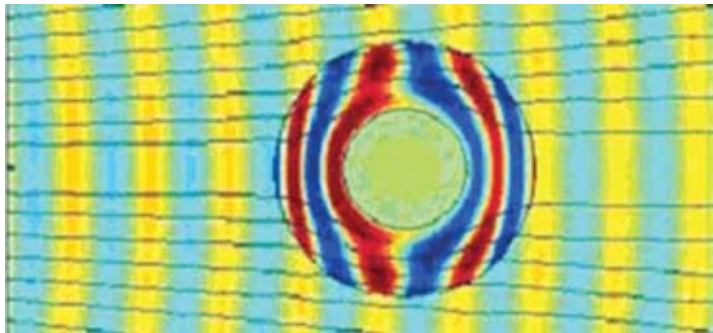
# 2. Design and perfect atom- and energy-efficient syntheses of new forms of matter with tailored properties

## Directing the "un-glueing" and "re-glueing" of electrons in reactions

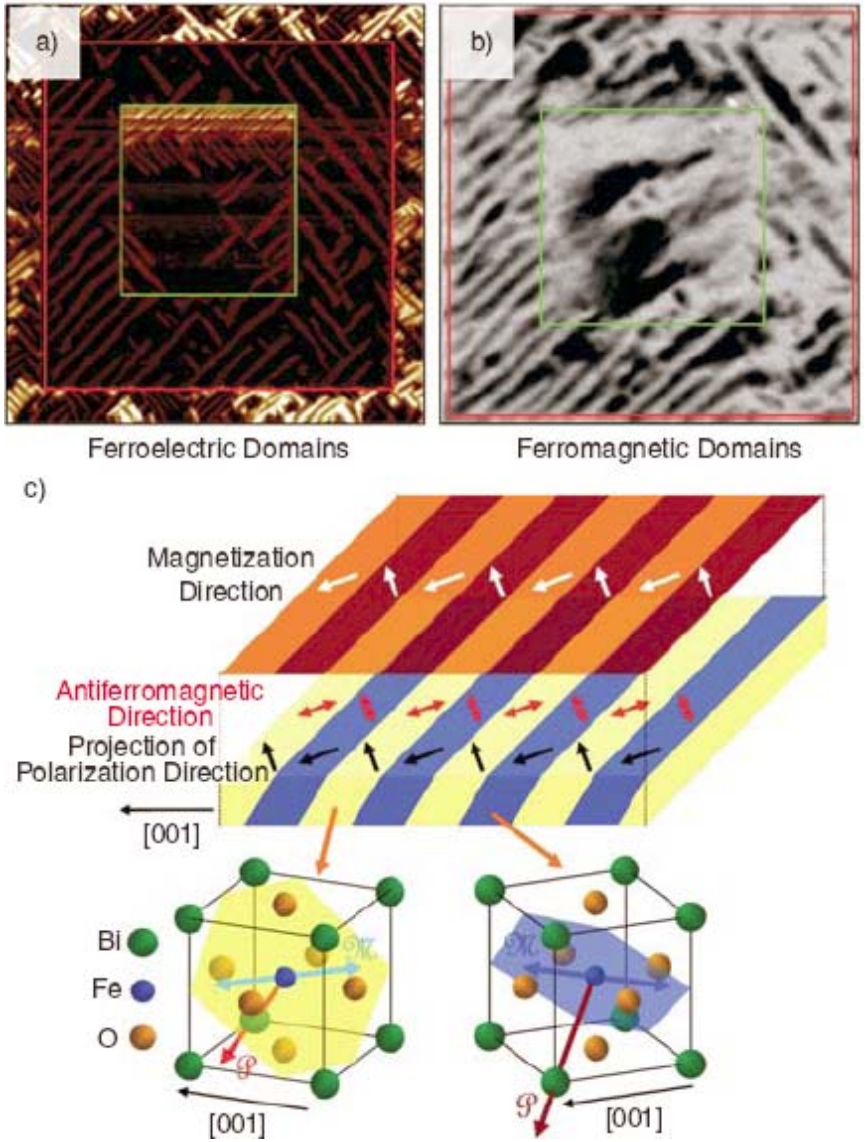


- Tailored new materials—only a tiny fraction of possible chemical compounds prepared
  - Self-regulation and self-repair of catalysts
  - Low cost, efficient solar cells
  - Molecular logic
- Directed synthesis guided by predictive design or reverse engineering
  - Design a particular electronic structure & find crystal structure and elements
  - Contra indicated properties (e.g. transparent conductors)
- Metamaterials: perfect lenses, invisibility cloaks



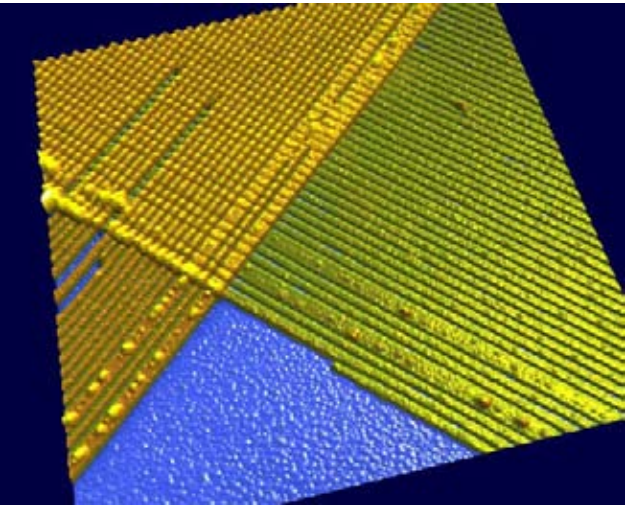
# 3. Understand and control the properties of matter emerge from complex correlations of atomic and electronic constituents




**Uncovering the fundamental rules of correlations and emergence and learning to control them**

- Emergent phenomena—correlated behavior can lead to unexpected collective outcomes
  - Superconductivity
  - Climate change
  - Cell colonies and soft matter
- Create information technology successor to semiconductors from strongly correlated materials
  - Magnetism
  - Ferroelectricity
- Quantum correlated liquids
  - Artificial photons and fractional quasiparticles
  - Error-free quantum computing

# 4. Master energy and information on the nanoscale



**Creating new technologies with capabilities rivaling those of living systems**

- Tap the existing world of biological nanotechnology by constructing interfaces between living cells and synthetic technology
- Fabricate devices with functionalities approaching those of living systems, but with different hardware implementation
- Nano-macro junctions: covering the gap from a few tenths to a few hundred nanometers (photonic, electrical & magnetic, mechanical)
- Defects and the end of Moore's law

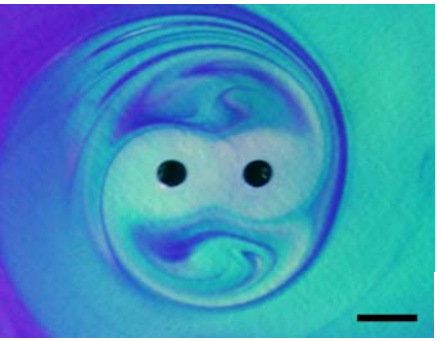
  *Adaptive probabilistic computing*
- Energy transduction at the nanoscale

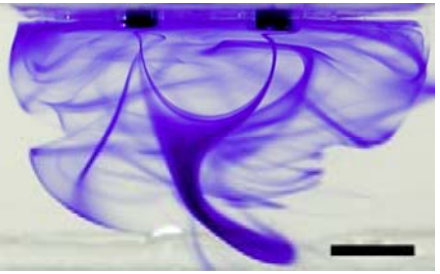
  *Stochastic processes, signals & noise*
- Ad hoc networking among nanoscale devices

# 5. Characterize and control matter away—especially very far away—from equilibrium

## Making non-equilibrium systems work for us

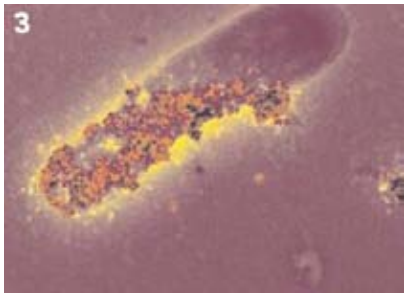
**Magneto-hydrodynamic self assembly**



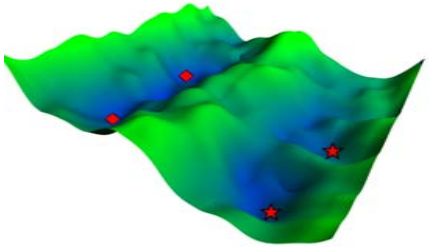


- Large range in scale
  - Microscopic (nano + bacteria)
  - Enormous (cyclone)
  - Time scales (ns to millennia)
- Nanoscale thermodynamics
- Exploration of free-energy landscapes
- Molecular transport junctions
- Fluctuations
  - Design, complexity, robustness
  - Energy-capture and energy-storage
- Jamming

**Shewanella**




**Molecular transport junction**



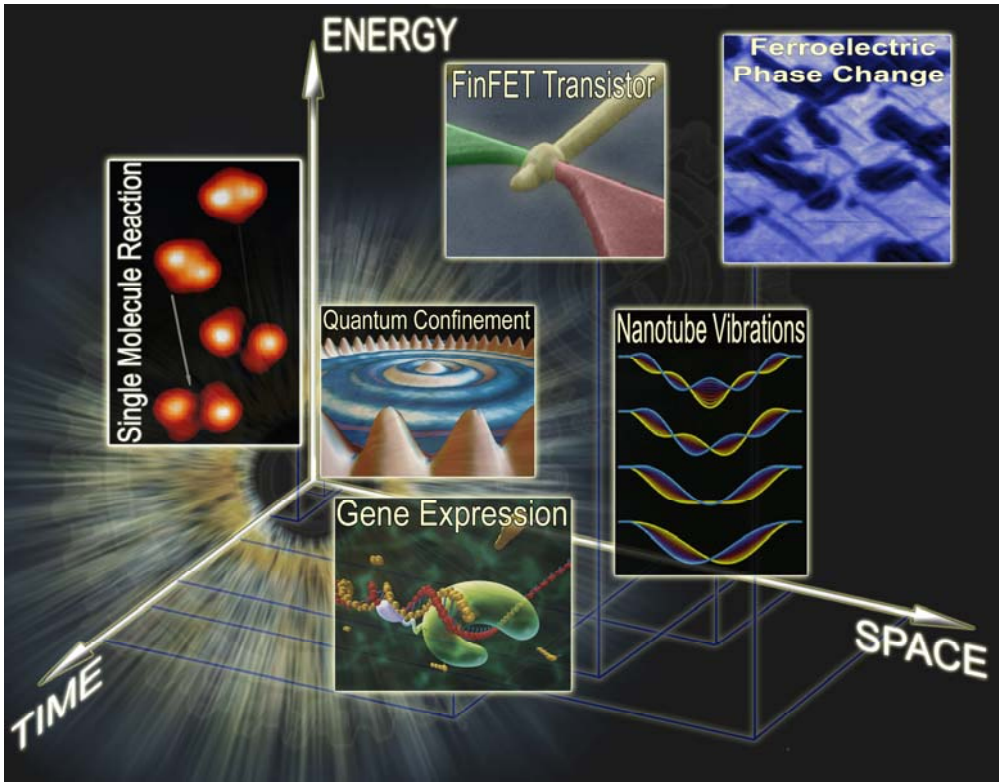
**cyclone**

# Overall Challenge: Making the Leap from Observation Science to Control Science

**The things we want to do—designing materials to have the properties we want and directing synthesis to achieve them—require the ability to see functionality at the relevant time, length and energy scales.**

**We will need to develop and disseminate new tools capable of viewing the <u>inner</u> <u>workings</u> of matter—transport, fields reactivity, excitations and motion ….**

**For example, a new generation of instruments will naturally lead to devices capable of directing matter at the level of electrons, atoms, or molecules.**



# What's Needed?

**The transition from <u>observation</u> science to <u>control</u> science envisaged in the five Grand Challenges requires a three-fold attack:**

(1) New approaches to training and funding

(2) Development of instruments that are more precise and flexible than those used for observation science

(3) Creation of theories and concepts beyond those we currently possess

Page 111, Grand Challenges Report

# 1. New Approaches to Training and Funding

**INNOVATION in basic energy science is critical to the nation and requires the engagement and support of our most creative scientists**

- **Sustained effort over long periods of time**
  - ***The DOE Energy Institute***
- **Awareness of the technological, industrial and policy implications**
  - ***The Energy Sciences Study Group***
- **Firmly anchored in one or two areas and able to communicate effectively across physics, chemistry, engineering, and biology**
  - ***The DOE Fellows Program***

# Next Generation Training and Funding: The DOE Energy Institute

- Modeled after HHMI investigators
- Energy Science Senior Fellows would have unrestricted, long-term support to allow the best minds to focus on Grand Challenge science and enhance the prestige and visibility of DOE Basic Energy Science Support
- Selection by blue–ribbon committee of DOE, national lab, and university leaders

Provide (for 5 years) part of normal year funding

# Next Generation Training and Funding: The Energy Sciences Study Group

- A two-year mentored program in energy policy, global energy needs, and related R&D
  - Mentors and advisors would come from the energy industry, energy and environmental policy
- Create a group of young faculty and national laboratory scientists
- Keep pace with evolving technology
- Convey understanding of the scientific and technical aspects of national energy security issues along with an appreciation of the multidisciplinary nature of energy research
- Lead workshops to define science challenges, underpinning energy and environmental issues, in conjunction with the Energy Sciences Network

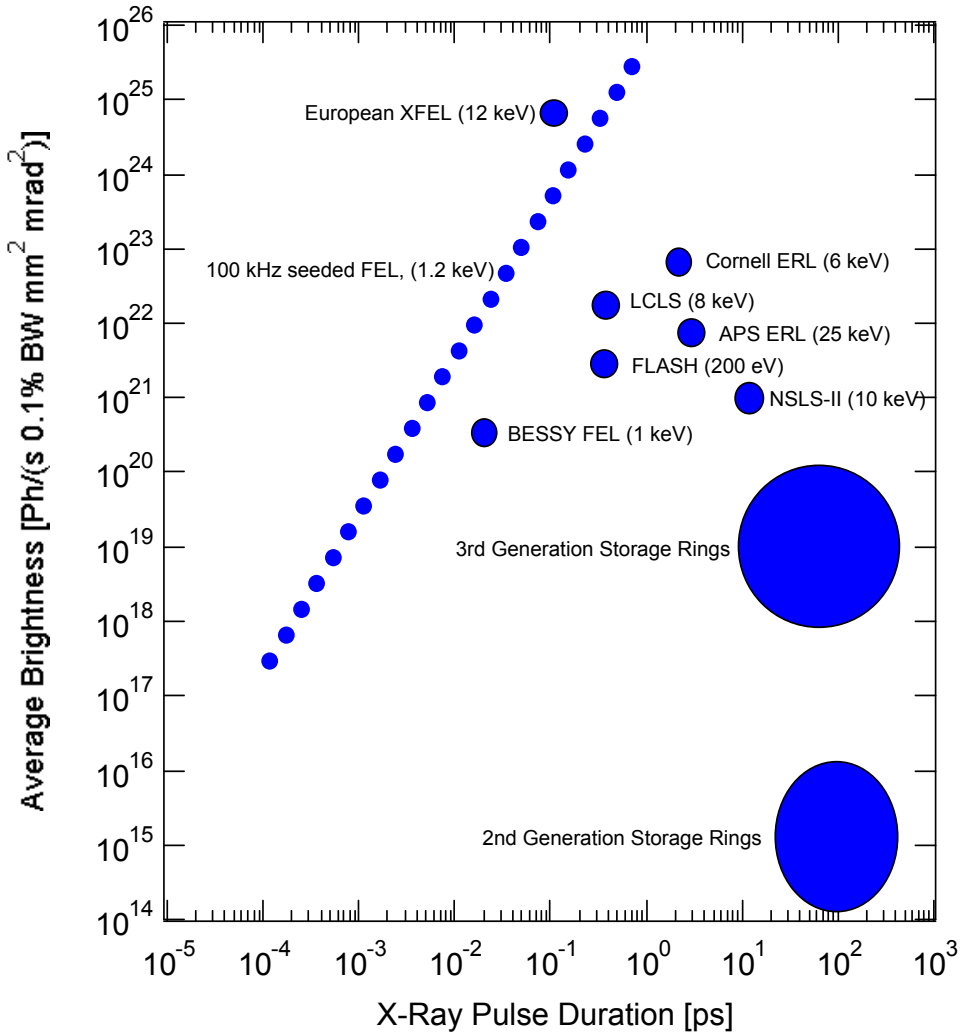
# Next Generation Training and Funding: The Energy Sciences Network

- Expand science training at Universities & Nanoscience centers (model: Cold Spring Harbor)
- Hold short series of Grand Challenge-focused workshops with two days of training in key issues for students followed by two days of forefront Grand Challenge science
- Create Grand Challenge Training Networks: collaborations between teams of scientists with early stage scientists spending time in more than one team
- Early stage scientists can
  - Customize their training
  - See multiple viewpoints
  - Begin their own collaborations

# 2. Next Generation of Instruments

- Requirements for Grand Challenge Science include:
  - Higher time resolution
  - Improved imaging methods
  - Improved and new kinds of detectors
  - Materials, especially crystal growth facilities
  - Computation and algorithm development
- Need: a balance between equipment for individual investigators, mid-scale and large-scale facilities
- A creative instrumentation program that supports design, construction and application of entirely new instruments
  - Single PI/small group level
- What machines could have the broad impact of synchrotrons?

# Next Generation of Instruments:
# Machines with Broad Impact of Synchrotrons



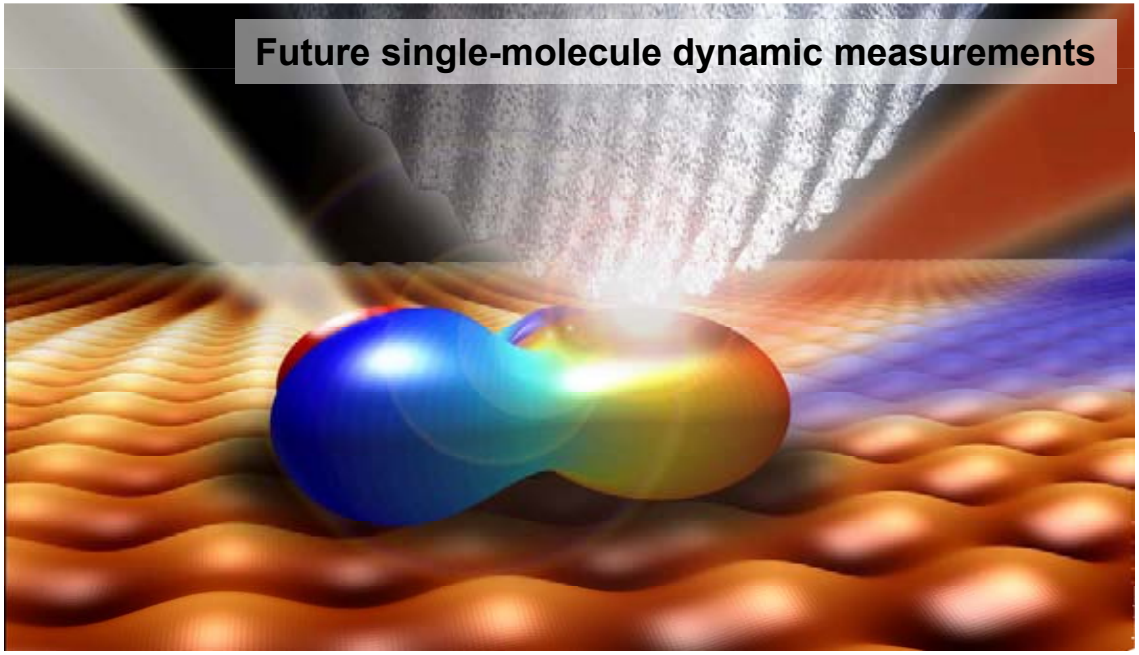

- **Higher time resolution**
- **Improved imaging methods**
- **Improved and new kinds of detectors**

***Average brightness versus pulse duration for storage ring, ERL, and FEL sources. Values are shown for optimized brightness at the photon energies indicated, based on available data.***

# Next Generation of Instruments:
# Sub-molecular Spatial & fs Time Resolution

**We must interrogate matter at a level much deeper than the macroscopic average to observe and control the properties of individual molecules or microscopic domains of materials**

**The biggest challenge lies ahead …**



# 3. Grand Challenges and Theory

**Theoretical challenges described in this report cannot simply be reduced to ever larger computations….**

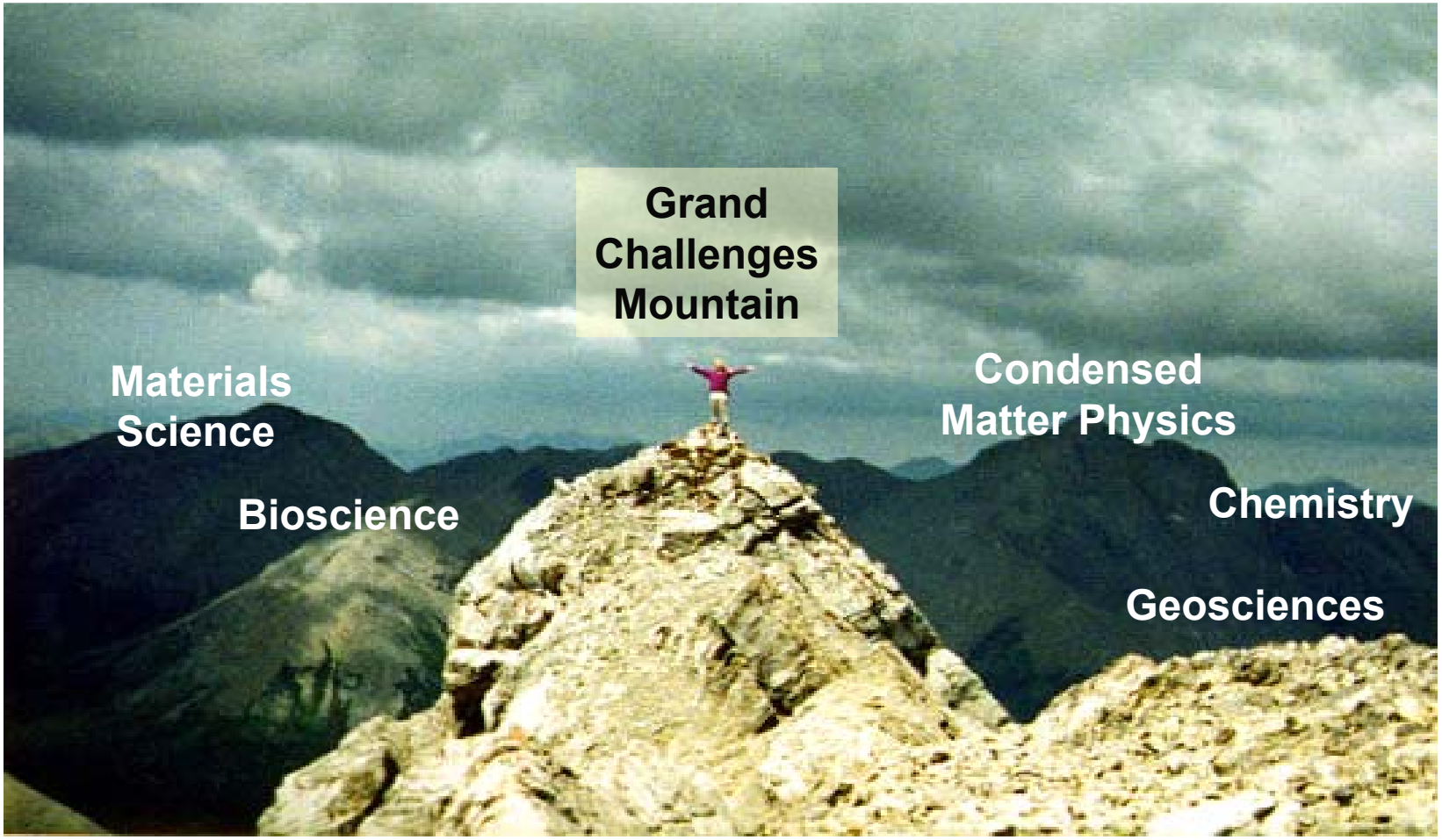
**…in many cases we do not know how to formulate theory well enough to compute anything**

- **We need to create a culture for high-risk, high-reward theoretical exploration of grand challenge topics (coherence, correlations, inter-conversion of energy and information, non-equilibrium phenomena)**
- **We need to attract the brightest, most theoretically inclined minds to basic energy sciences**

# Energy Scientists of the Future

**"Energy is at the core of virtually every problem facing humanity. We cannot afford to get this wrong."**

**-R. Smalley**



# Grand Challenge Science

**"These capabilities will <u>transform</u> basic energy sciences, play a critical role in securing our energy future, and produce applications not yet imagined."**

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# Top 10 Challenges: Next 50 Years

1. ENERGY
2. WATER
3. FOOD
4. ENVIRONMENT
5. POVERTY
6. TERRORISM & WAR
7. DISEASE
8. EDUCATION
9. DEMOCRACY
10. POPULATION

| | | |
|---|---|---|
| 2003 | 6.3 | Billion People |
| 2050 | 8-10 | Billion People |

Source Richard Smalley Energy & Nanotechnology Conference
Rice University, Houston May 3, 2003