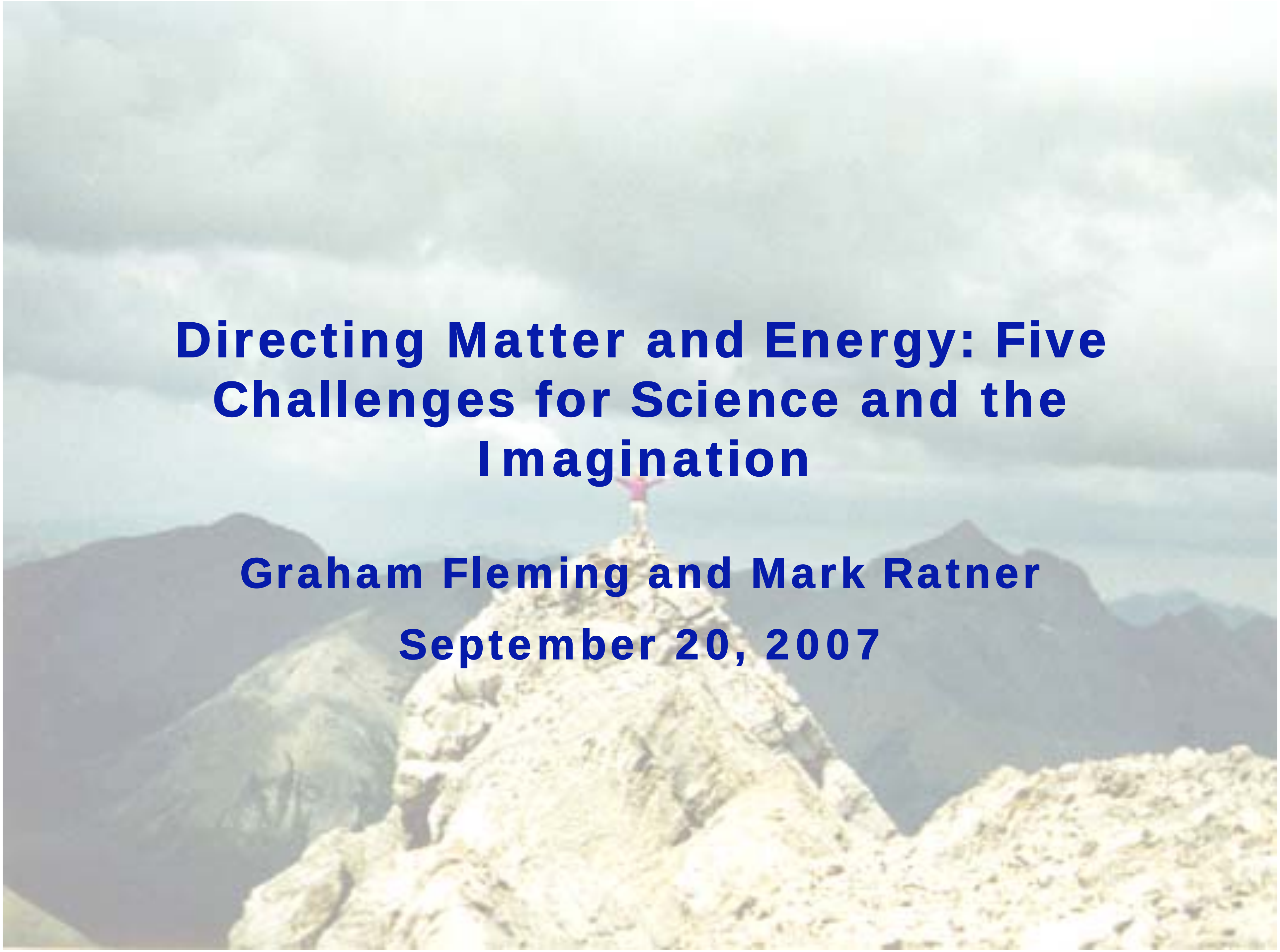


Directing Matter and Energy: Five Challenges for Science and the Imagination

Graham Fleming and Mark Ratner

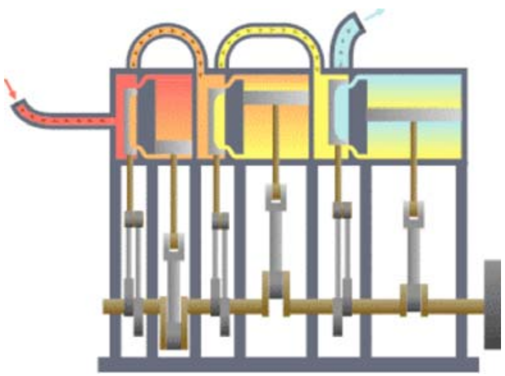
September 20, 2007

Why Grand Challenges Now?
Observation to Control

19th Century

Average Behavior
of Continuous Systems

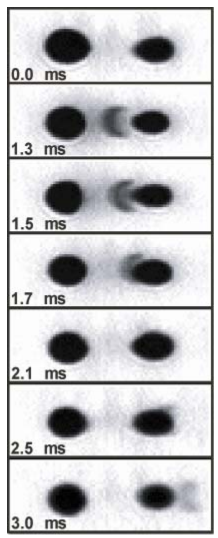
Thermodynamics



20th Century

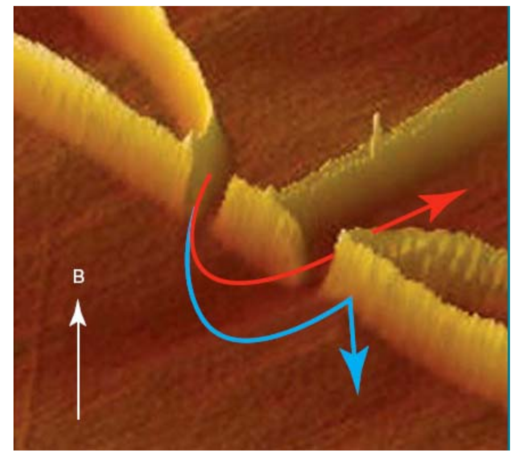
Discrete and
Fluctuating Systems

Functional Units
Quantum Mechanics



21st Century

Control **of Matter & Energy**



"During the 20th century, scientists developed increasingly sophisticated technologies and instrumentation for the study of quantum effects. Our understanding of these phenomena has reached the point where we are ready to move beyond simple observation and take the steps that will enable us to direct and control matter and energy at the quantum level."

--Grand Challenges report , Chapter 1

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?

Winnowing the Grand Challenges

Certain scientific areas were re-occurring when….

1) we go to the *<u>very</u>* small

2) we go *<u>far</u>* from equilibrium

3) we encounter strongly correlated systems & systems with emergent properties

4) we want to define the limits of material properties

5) we want to manipulate energy and information ever more rapidly and efficiently

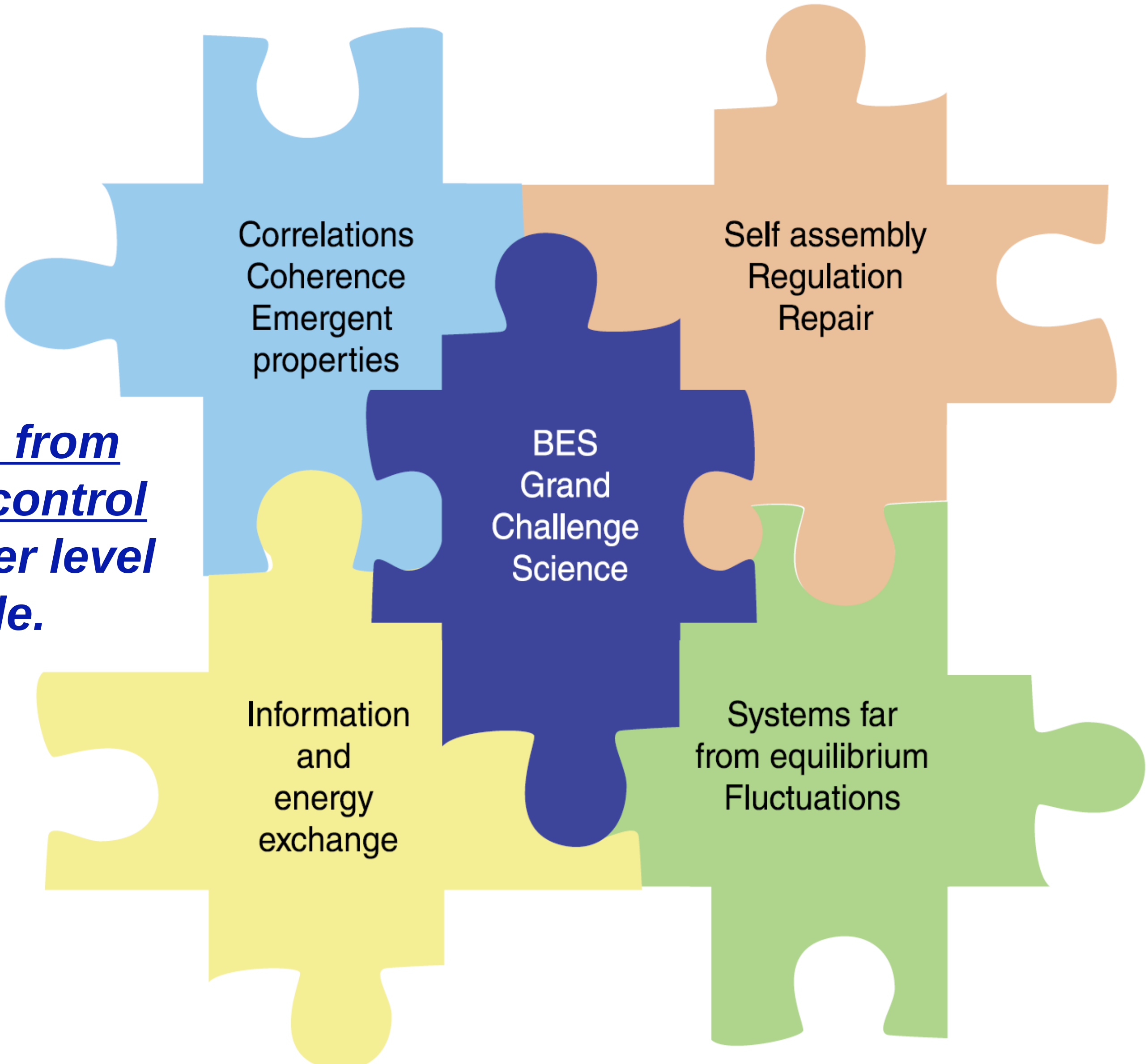
6) we want to recreate in synthetic systems properties and capabilities we find in nature

Connecting Themes

An underlying set of concepts emerged.

Our ideas suggested that 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.

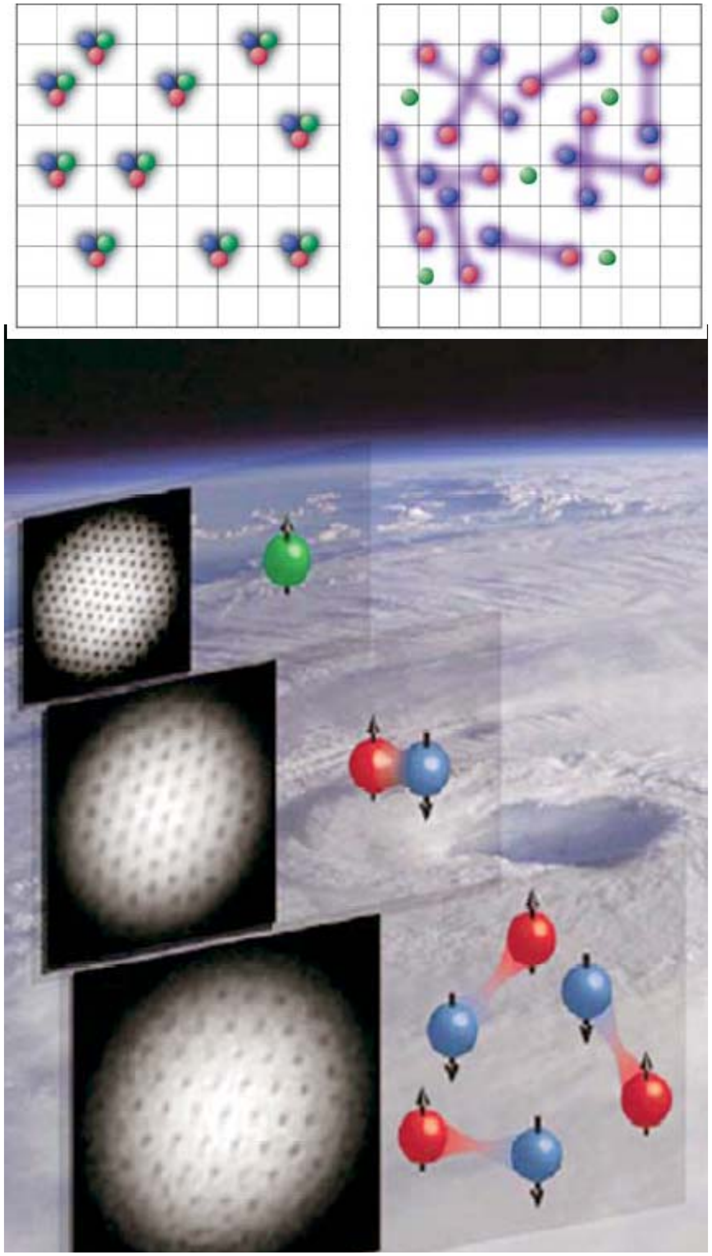
These two ideas led us to construct five large challenges.



Five Grand Challenges for Science and the Imagination

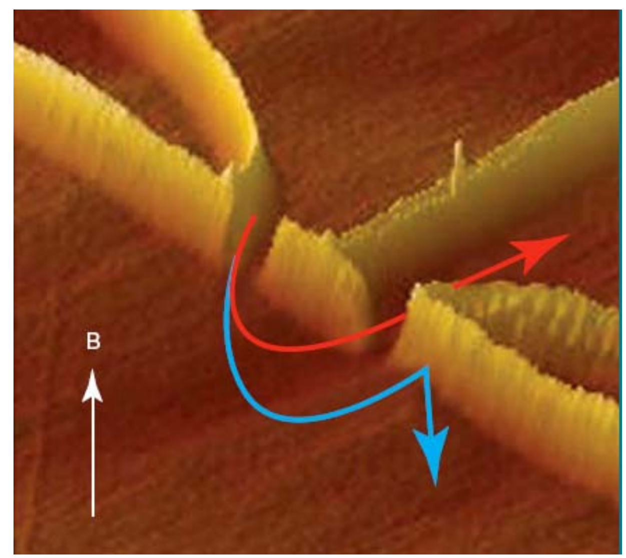
- ***How do we control materials and processes at the level of electrons?***
- ***How do we design and perfect atom-and energy-efficient synthesis of new forms of matter with tailored properties?***
- ***How do remarkable properties of matter emerge from complex correlations of atomic and electronic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

Grand Challenge: ***How do we control materials and processes at the level of electrons?***



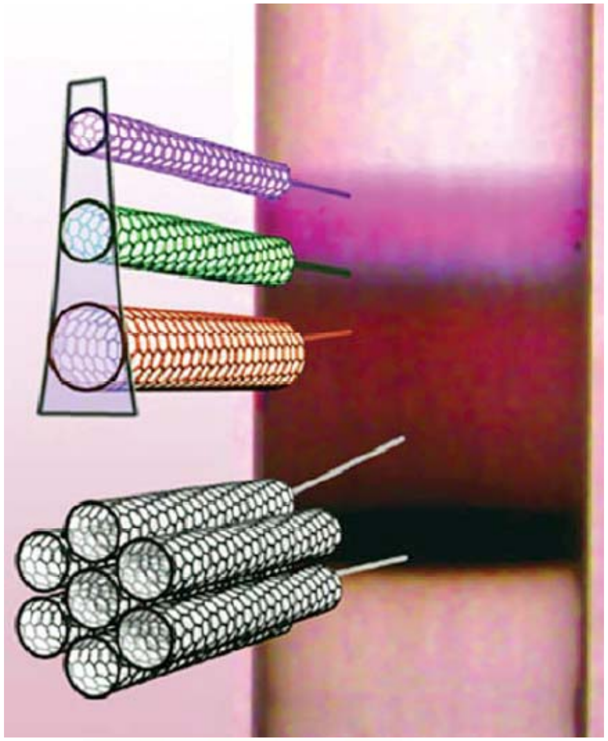
Making quantum systems work for us

- Attosecond optical pulses, high intensity excitation
  - --Failure of Born-Oppenheimer Approx.
  - --Conical intersections
- Control of spins (spintronics)
- Quantum computing and the use of coherence in devices.
- Quantum simulators

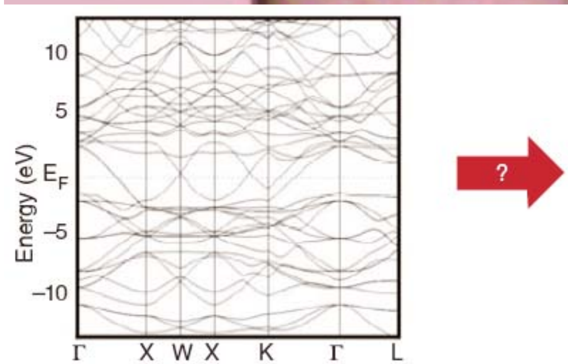


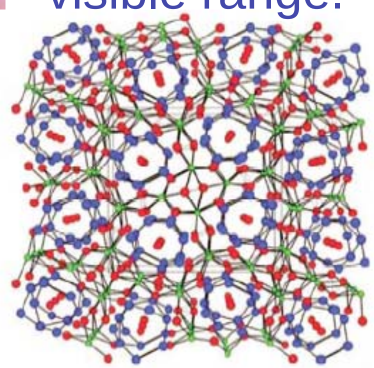
Grand Challenge: *How do we design and perfect atom- and energy-efficient synthesis of new forms of matter with tailored properties?*

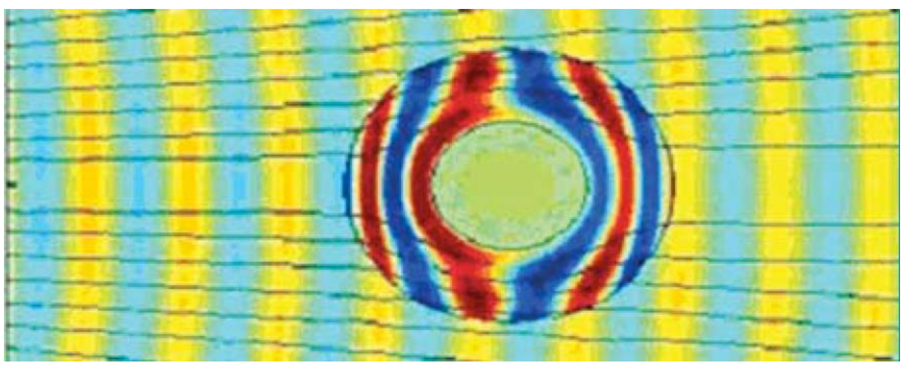
Directing the "un-glueing" and "re-glueing" of electrons



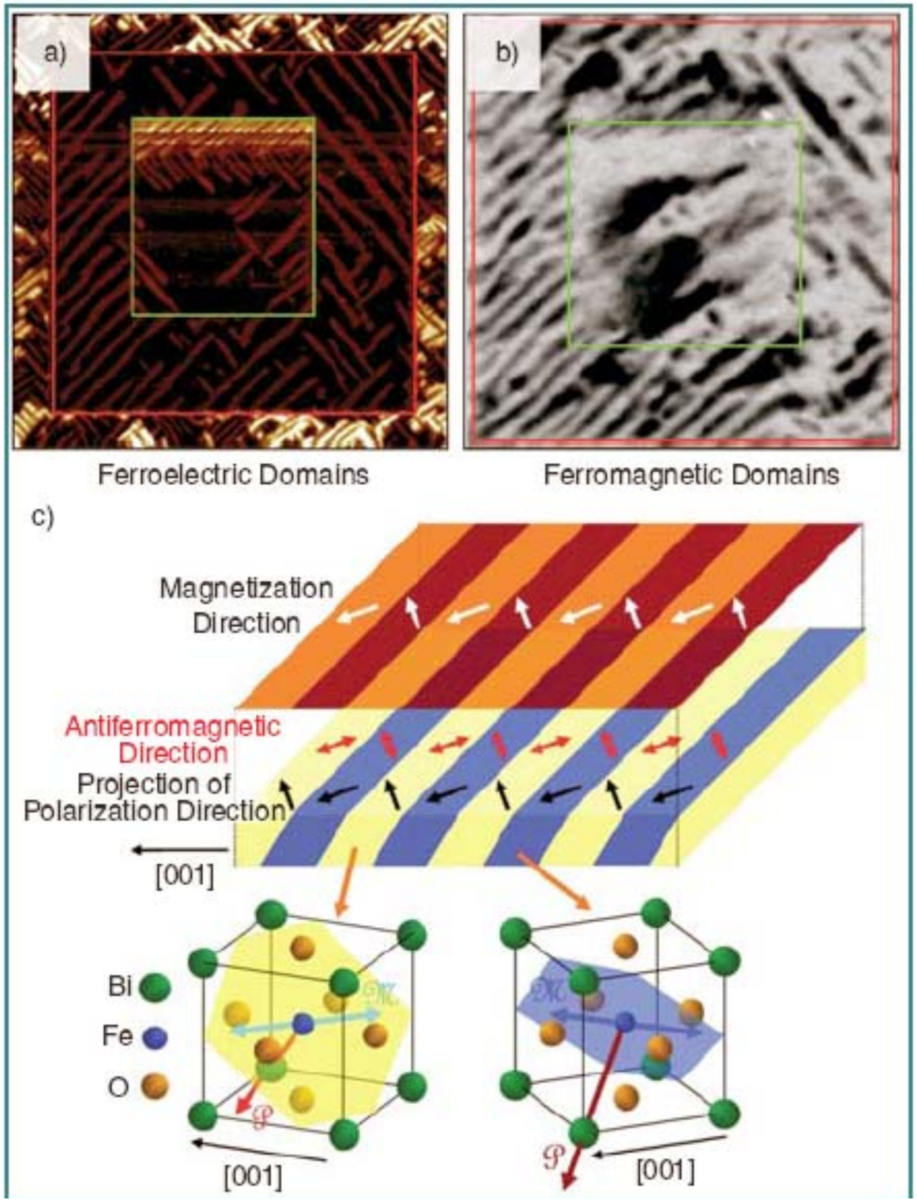
- Design for a particular electronic structure by finding the optimum combination of crystal structure & elements that yields (e.g. a specified band structure).
- Design for self regulation and even self repair of catalysts
- Low cost efficient solar cells
- Designing molecular logic
- Contra indicated properties (e.g. transparent conductors).
- Meta materials: perfect lenses, invisibility cloaks in the visible range.







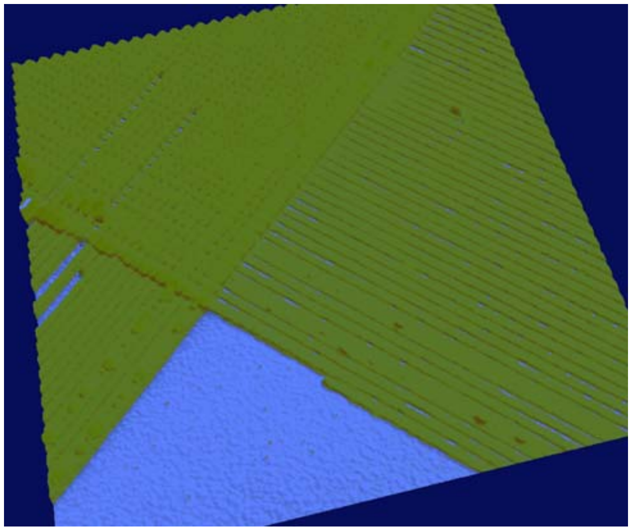
Grand Challenge: *How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties?*

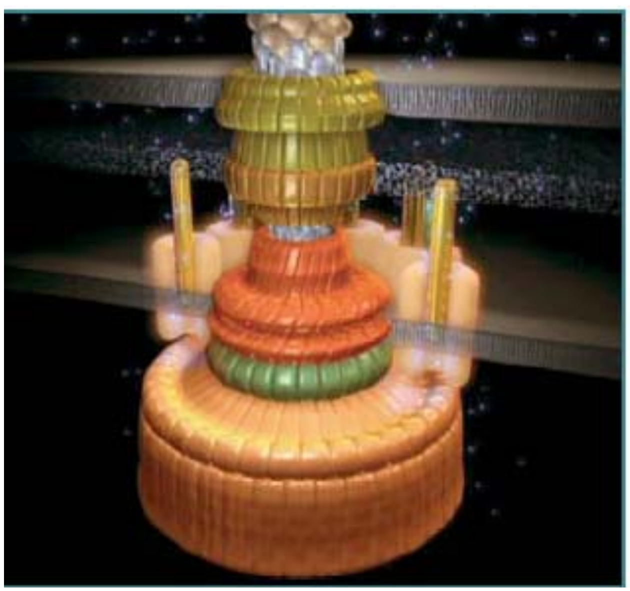


Uncovering the fundamental rules of correlations and emergence & learning to control them

- Create successor to current semiconductors from strongly correlated materials (e.g. multiferroics combine and couple electric & magnetic action—electrical control of magnetism)
- Quantum correlated liquids
  --Quantum spin liquids: artificial photons, fractional quasi particle (error free quantum computing)
- Strongly correlated atoms
  --quantum emulators & simulators (e.g. tests of the Hubbard Model for cuprates)
- Soft matter
- Biology

Grand Challenge: *Can we master energy and information on the nanoscale?*



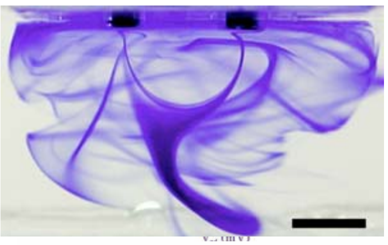


Creating new technologies with capabilities rivaling those of living systems

- 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

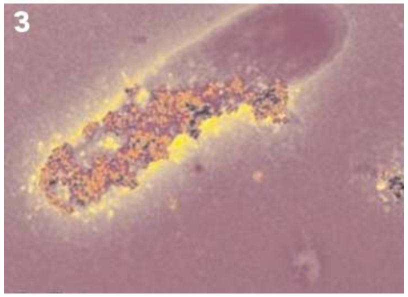
Grand Challenge: *How do we characterize and control matter away—especially very far away—from equilibrium?*

Magnetohydrodynamic self-assembly

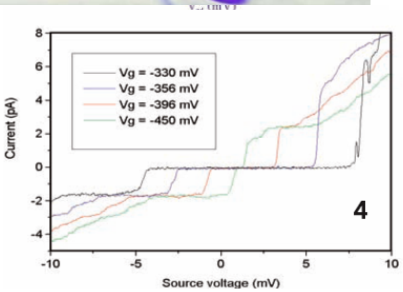


Making non-equilibrium systems work for us

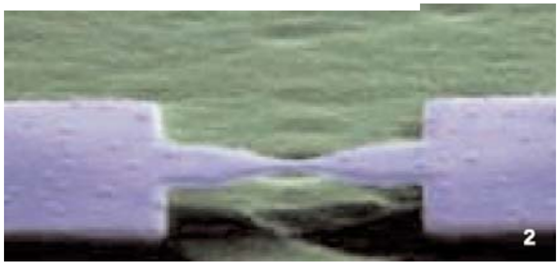
- Nanoscale thermodynamics
- Molecular transport junctions
- Fluctuations; Design, complexity, robustness
  - --energy-capture & energy-storage capabilities, mitigate environmental damage
- Exploring rough landscapes
- Jamming
- Science of life

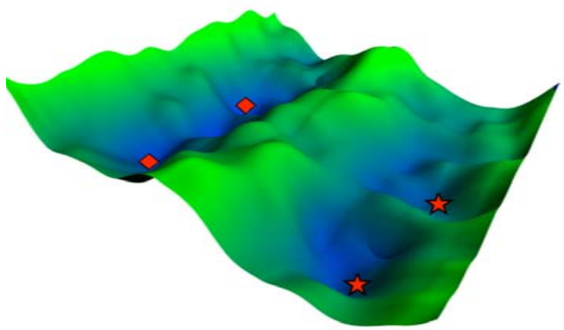


Shewanella



Molecular transport junction





cyclone

What's Needed?

The transition from observation science to control science envisaged in the five Grand Challenges requires a three-fold attack: new approaches to training and funding, development of instruments that are more precise and more flexible than those used for observation science, and creation of theories and concepts beyond those we currently possess.

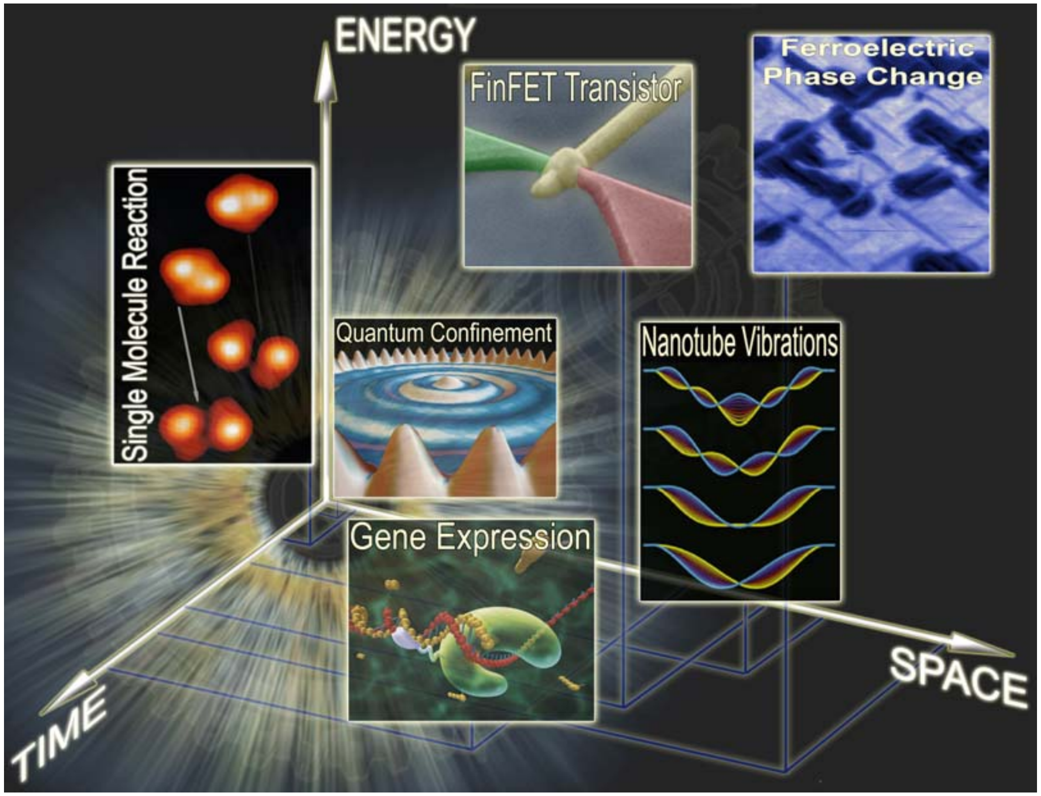
Page 111, Grand Challenges Report

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

The things we want to do (i.e. designing materials to have the properties we want & directing synthesis to achieve them) require the ability to see functionality at the relevant time, length & energy scales.

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

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



21st Century Light Sources:

An assessment of needs driven by new scientific opportunities

- The BES suite of storage-ring-based light sources is one of the largest and most scientifically productive complex of user facilities in the world, serving more than 8,500 users each year.
- The Linac Coherent Light Source at SLAC, the first hard x-ray, linac-based light source, will be added to this complex in FY 2009. It will be fully operational a year or two later.
- The National Synchrotron Light Source – II at BNL, an advanced ultra bright storage-ring-based light source, will be added to the complex a few years later, in approximately 2015.
- By 2015, with LCLS and NSLS-II newly operating, the youngest of today's BES light sources will be approaching its 20th birthday. Now is the time for DOE and the scientific community to begin the process of strategic planning for the 21st century light sources that will be as impactful as today's light sources and address the scientific needs of the community in the 21st Century.
- The scientific opportunities and mission needs – as developed over the past five years in ten Basic Research Needs workshops and in the BESAC Grand Challenges study – are the major drivers for the specifications of new and upgraded light sources.

BESAC Charge

Consider the characteristics of the next generation light sources that will address the scientific and technological challenges put for in the Basic Research Needs workshops reports and the BESAC Grand Challenge study and that will enable new and innovative ways of probing our material world in the 21st Century.

The characteristics to be specified are the standard ones used to describe light sources: wavelength, flux, brightness, emittance, coherence, pulse length, potential instrument suite, availability and reliability of the entire system, and user accessibility. The charge excludes consideration of the many specific pre-proposals or proposals for light sources that are currently being discussed in the community. However, the capabilities of various types of light sources (including lasers, storage-ring-based and linac-based light sources, or other types of light sources) should be evaluated against the preferred characteristics of the new light sources. Both upgrades and new facility concepts may be considered in this context.

The work of the BESAC subcommittee should be reported to BESAC at its summer 2008 meeting.