Mesoscopic Materials and Chemistry

George Crabtree
ANL/UIC

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Charge

Committee

What is Meso?

Energy, length, time, complexity, functionality

Facilities and tools

Website for Input

Strategic Planning Meeting
Materials Science Division
Argonne National Laboratory
February 3, 2012

The BESAC Charge on Mesoscale Science

Excerpts from Dr. Brinkman's charge letter:

A central theme of these reports is the importance of atomic and molecular scale understanding of how nature works and how this relates to advancing the frontiers of science and innovation. I would now like BESAC to extend this work by addressing the research agenda for mesoscale science, the regime where classical, microscale science and nanoscale science meet. I see two parts to this new study:

1. Identify mesoscale science directions that are most promising for advancing the Department's energy mission.
2. Identify how current and future BES facilities can impact mesoscale science.

This study could prompt a national discussion of mesoscale science at the level heard during the initial formulation of the National Nanotechnology Initiative a decade ago.

Report due early Fall 2012

The BESAC Meso Subcommittee

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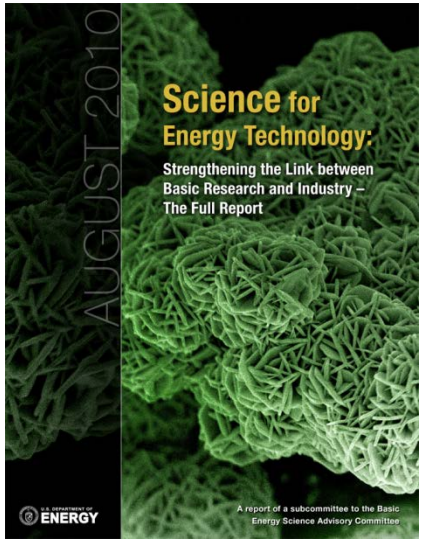
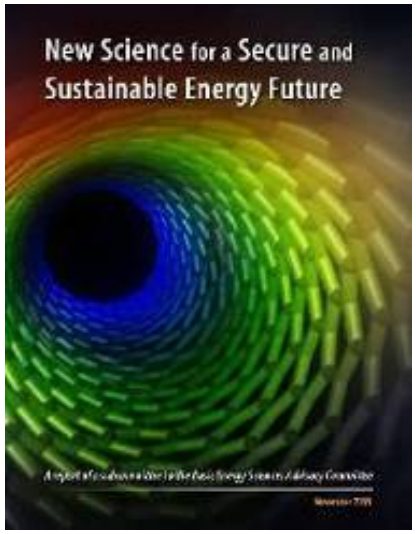
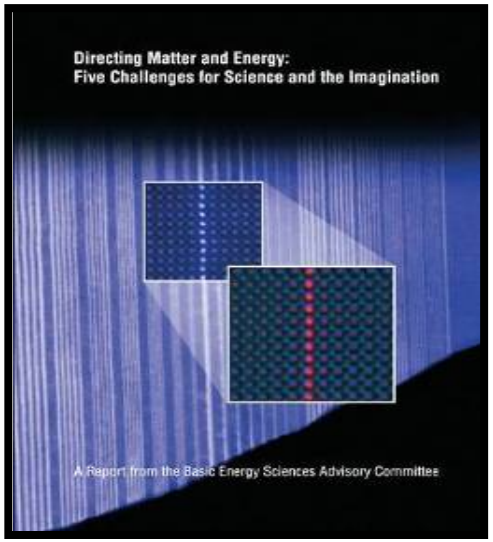
Eric Rohlfing, BES
Harriet Kung, BES

Relevant Background

- Why: the need for innovation, as articulated in e.g., Sci Tech report
- Why now: the insights and tools we've gained (and are still gaining) from nano, as articulated in e.g., New Era report
- What: build on the science challenges, as articulated in e.g., Grand Challenge report







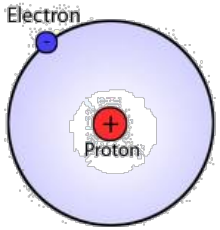
What is Meso?

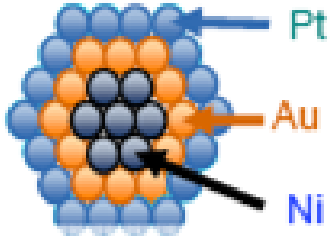
What is Meso?

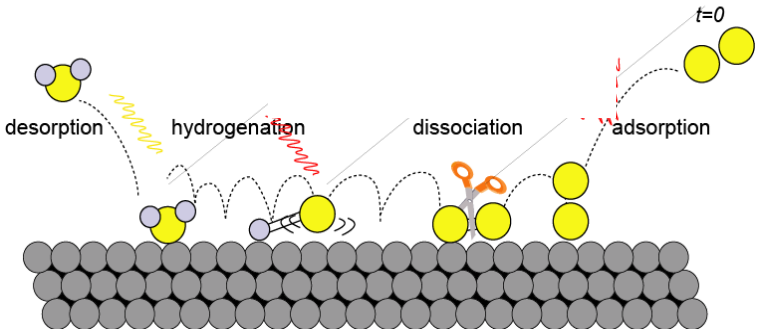
From the Greek

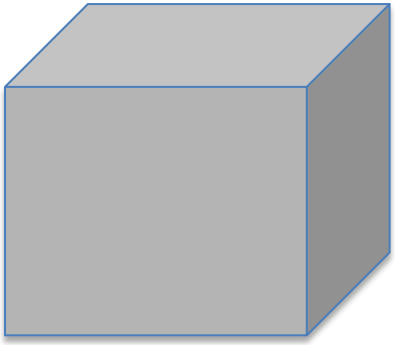
In between, intermediate, middle

Relative, not absolute







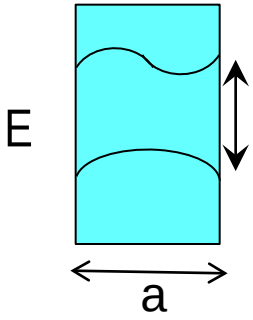


atomic

meso

bulk

What is Meso? An Energy Scale of Mixing



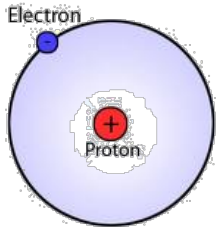
$\Delta E \sim n^2h^2/8ma^2$

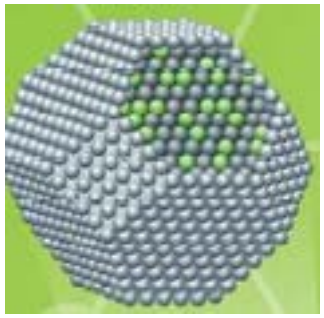
energy states mixed
by thermal fluctuations

$\Delta E \sim kT$ or h/τ

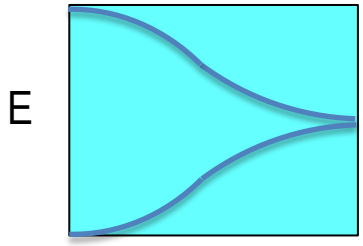
~ .025 eV
~ 300 K

$\Delta E = 13.6$ eV





$\Delta E \sim 0$

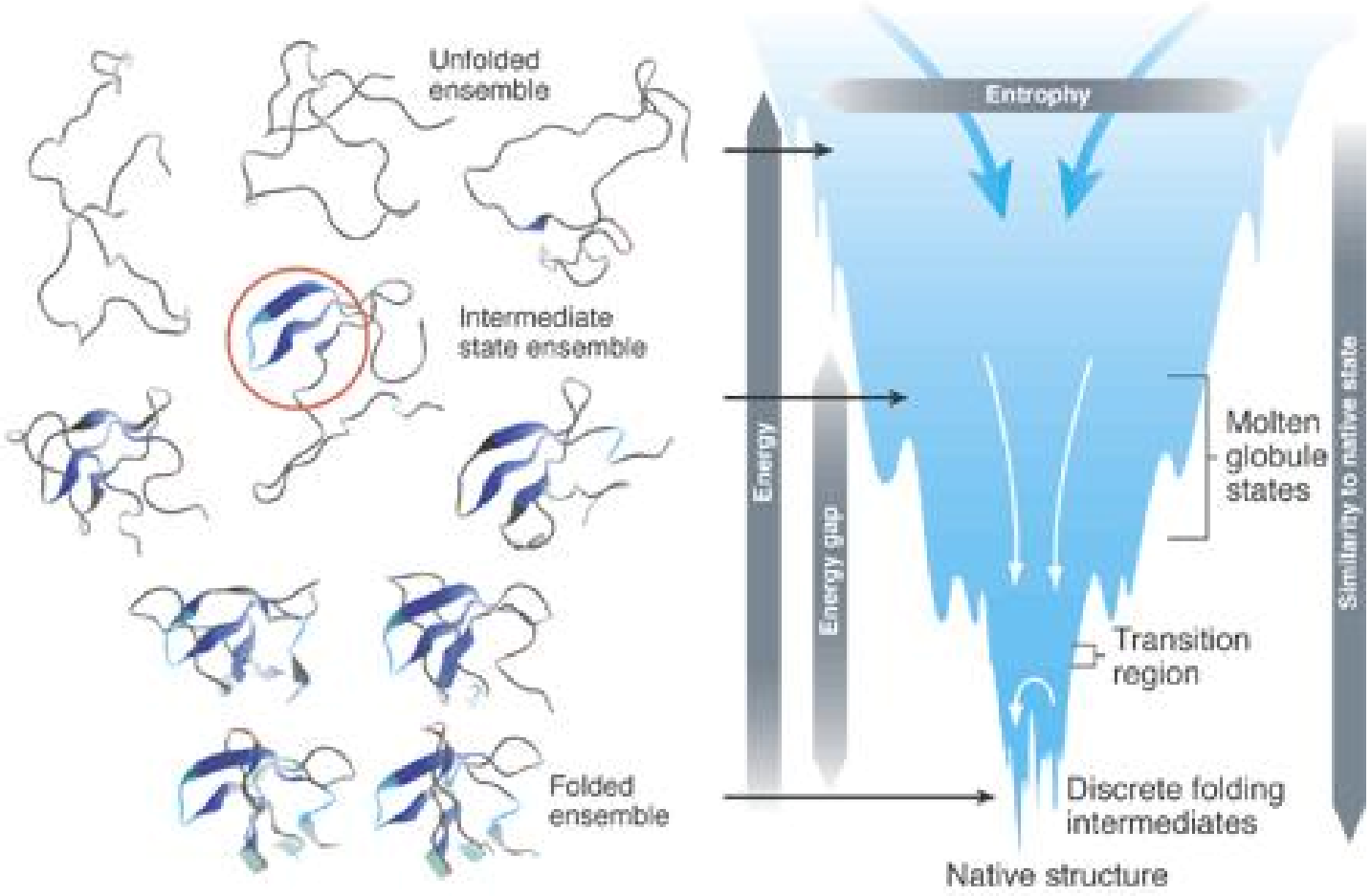


quantum — continuous

atomic	meso		macro
0.1 nm	10 nm	100 nm	1000 nm
10^{-10} m	10^{-8} m	10^{-7} m	10^{-6} m

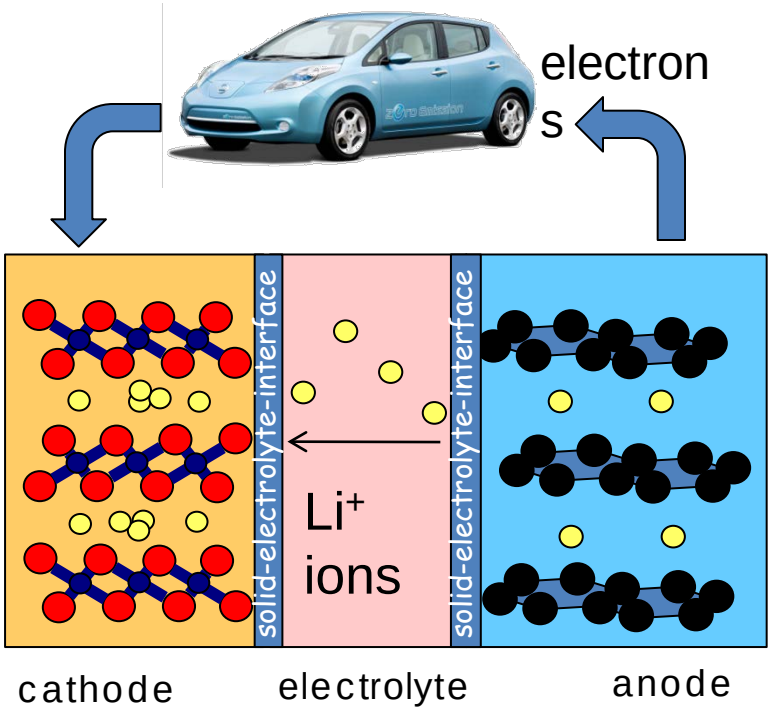
Self-assembly by Thermal Mixing of Energy Levels

Protein Folding



http://www.biology-online.org/articles/statistical_thermodynamics_taking_walk.html

What is Meso? Interacting Degrees of Freedom



Phenomena
Ionization
Ion insertion/extraction
Electronic / ionic conduction
Volume expansion/contraction

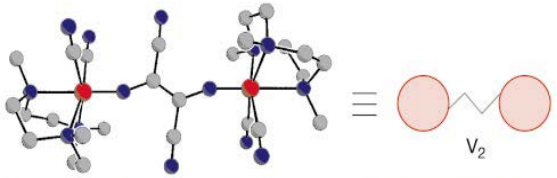
Degrees of freedom
Electronic
Ionic
Chemical
mechanical

Functionality
Energy storage
Energy delivery
Reversibility on demand

What is Meso? The Gap between Top Down and Bottom Up

Top down lithography to 10 nm
remove material without atomic control

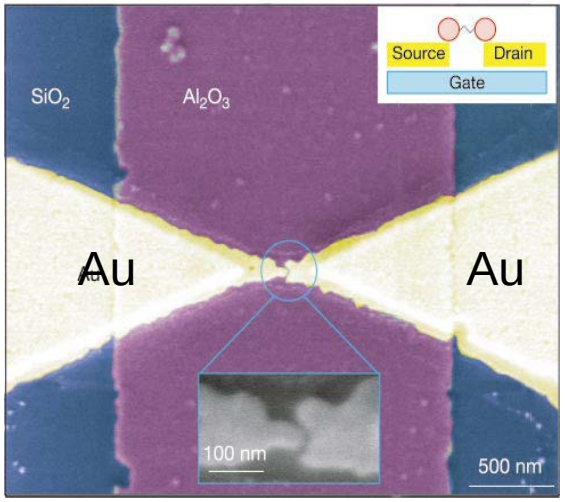
Bottom up self-assembly from atomic and molecular scales
build atom by atom placements



Single molecule transistor

Top down contacts to bottom up functional unit

Challenge:
Connect chemical and electronic energy levels



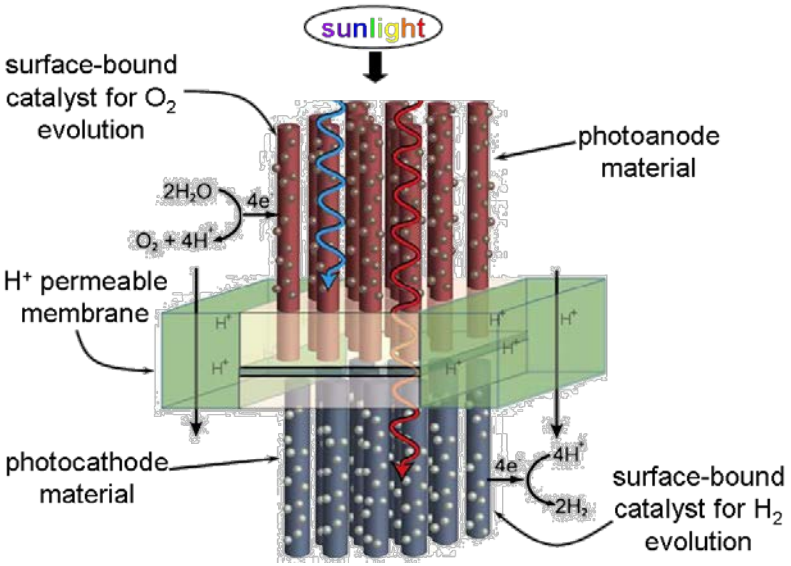
Wenjie Liang, Matthew P. Shores, Marc Bockrath, Jeffrey R.Long & Hongkun Park, Nature 417, 725 (2002).

"wiring up the nano world"

Quantum dots and molecular electronics

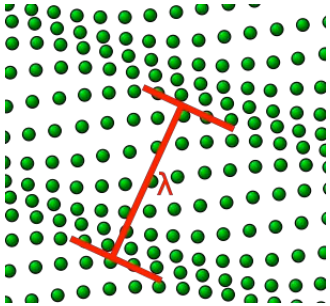
External communication with Internal energy levels

What is Meso? A time scale for each degree of freedom



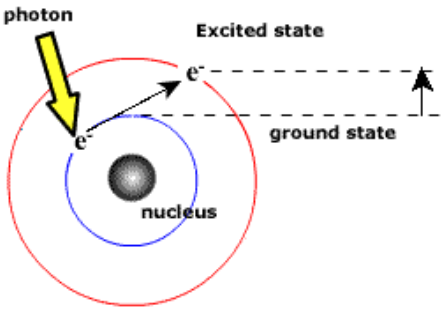
http://ccisolar.caltech.edu/webpage/95

Solar water splitting system

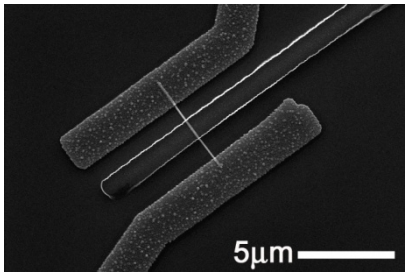


Mechanical deformation
10 fs - 10 ps

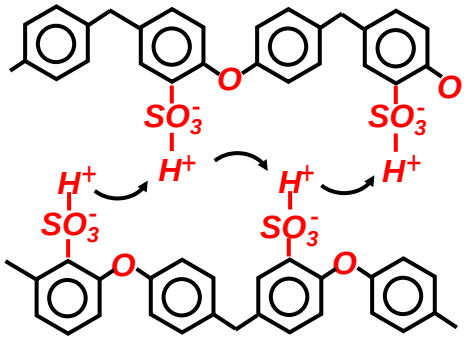
Electronic excitation
100 as



Electronic conduction
100 fs



Ionic conduction
10 ps



Mesoscale phenomena and functionality
All time scales contribute

What is Meso? An opportunity space

At the meso scale, multiple degrees of freedom interact constructively:

- Complexity enables new phenomena and functionality
- Consilience of systems and architectures
- Biology is an inspiration and proof of principle
  - Biological complexity with inorganic materials

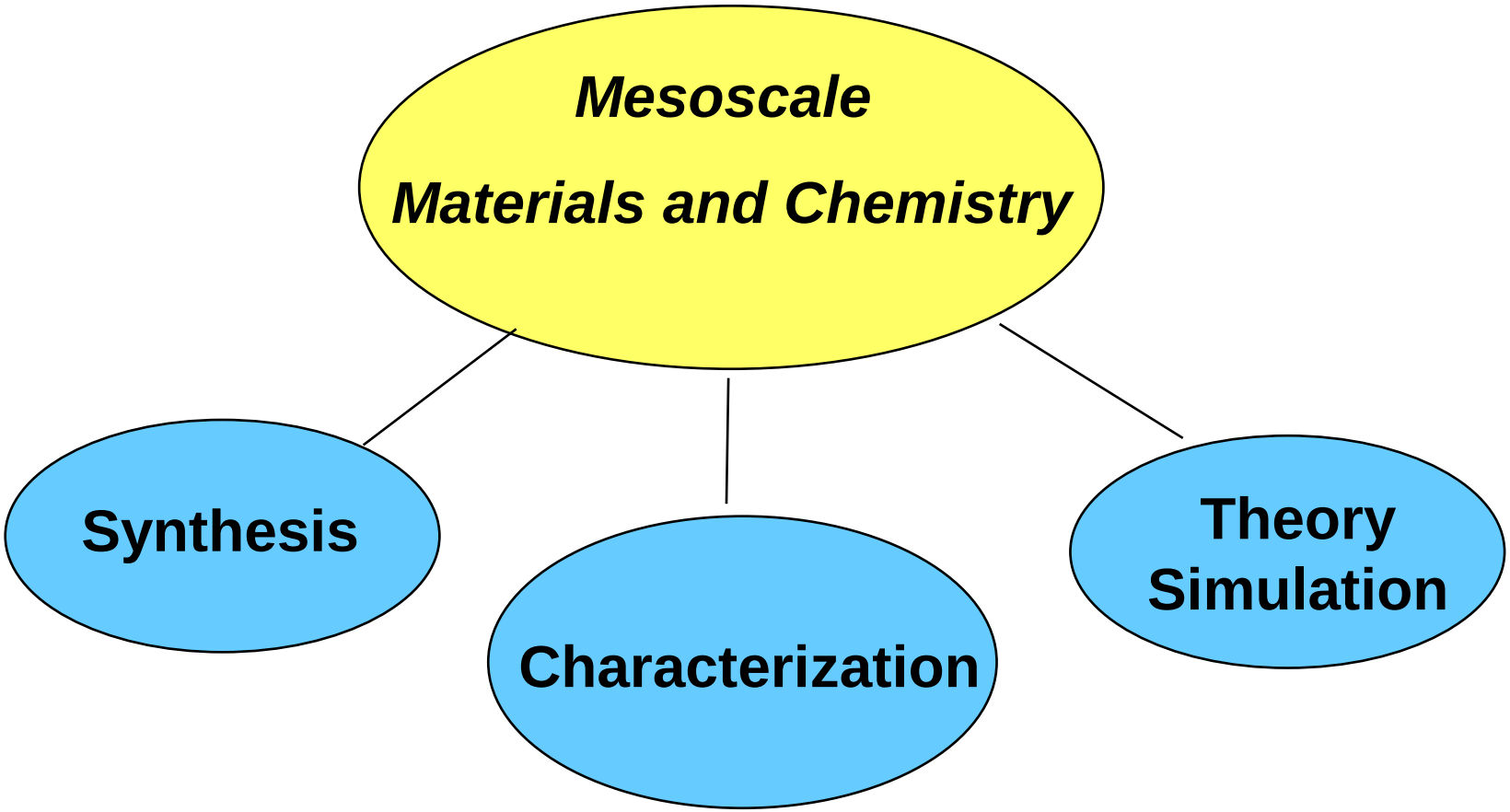
At the meso scale, multiple spatial and temporal scales meet:

- Quantum gives way to classical
- Top-down meets bottom-up
- Equilibrium is irrelevant: kinetics count

At the meso scale, new organizing principles are needed

- Meso is beyond reductionist science
  - What laws govern self-assembly?

Realizing the Meso Opportunity: Integration across Tools and Facilities



Supercomputing Facilities, Light Sources, Neutron Scattering Facilities,
Electron Beam Microcharacterization Centers, Nanoscience Centers

Meso Tools and Facilities

Synthesis

- Rational synthesis of inorganic materials with lessons of organic chemistry in complex materials
- Intrinsic complexity of materials at meso scale → Ultraclean for bottoms up → multi-step assembly→ sequencing of processes→ ultradirty facilities
- Synthesis that can scale to manufacturing
- Capacity/Capability to make populations/ensembles of samples

-Need for model systems

Characterization

- In situ and real time measurements
- in operating environments, non destructive, in vivo
- Multi-modal experiments, e.g. structure + excitation
- Consider statistical variation of complex meso samples
- Raw data vs analysis/interpretations; statistically significant results vs observations
- 4d materials science
- Faster processes/increased availability (e.g., fib/ serial sectioning, etc.; larger fields of view)
- Measurement induced damage considerations (beyond probe and destroy)
- Time scales attosec to decades

Theory and Computation

- New organizing principles
- Beyond average behavior, and perfect periodicity
- Spatially resolved measurements
- Theory and expt in the same conditions
- Understand ramifications of measurements (what is really being measured, esp given complexity)
- Simulate synthesis outcomes
- Simulate functionality of composite systems

Integration

- Synthesis ←→ Characterization ←→ Theory/Simulation
- Multiple simultaneous/concurrent measurements, **including across length & time scales**
- Complete suite of measurements on same/similar samples
  - including sample transport/interchangability between beam lines
- Co-design of experiment and simulation

Priority Directions/Key Themes –working titles based on initial meeting

Damage Accumulation and Materials Lifetime

Functional Mesoscale Systems

Self and guided assembly in biology

Reactive transport through mesoporous media

Role of fluctuations in formulating organizing principles in meso-scale systems

TOPICS TO FURTHER ELABORATE
Electromagnetic phenomena

Catalysis

Non-living organic matter; health effects

(INSERT TITLE)

Opportunity

Brief overview of the underlying scientific challenge/current state of understanding

Approach

What can be done to address the challenge? What are the key steps along the way?

What new tools and techniques need to be developed to address the challenge?

Meso Challenge

What makes it meso?

Impact

How will pursuit of the research direction, including the meso opportunity, impact the scientific challenge?

References:

Mesoscale Priority Research Direction

Self-assembly of Inorganic Nanoparticles

Opportunity

Self-assembly of inorganic nanoparticles into larger architectures creates composite functionality and new phenomena of strong basic and applied interest. Architectures can be periodic or glassy, composed of one or various nanoparticle constituents, and extend in 1,2 or 3 dimensions. Phenomena include photonic, electronic, magnetic, catalytic, and acoustic behavior.

Meso Challenge

The challenge is to identify the architectures and compositions that lead to targeted mesoscale phenomena and functionalities, then direct self-assembly to express the desired architecture.

Approach

Various assembly approaches are possible, utilizing electrostatic interactions, dipole attractions, van del Waals forces, hydrogen bonding and hydrophilic/hydrophobic interactions. Polymers or DNA templates that are later removed can force metastable architectures; temperature and laser excitation can be used to promote or limit kinetic exploration of complex assemblies.

Impact

Self-assembled inorganic nanoparticles promise a host of new mesoscale phenomena and functionalities that require minimal material and thus reduce cost, place functional units in close proximity and thus increase speed and efficiency, and provide qualitatively new routes to targeted outcomes.

M. Antonietti and G.A. Ozin, *Promises and Problems of Mesoscale Materials Chemistry or Why Meso*?, Chem. Eur. J. 10, 28 (2004)

F. X. Redl, K.-S. Cho, C. B. Murray, S. O'Brien, *3D binary superlattices of magnetic nanocrystals and semiconductor quantum dots*, Nature 423, 968 (2003)

I. S. Beloborodov, A. V. Lopatin, V. M. Vinokur, K. B. Efetov, *Granular Electronic Systems*, Rev. Mod. Phys.79, 469 (2007)

Y. Gao and Z. Tang, *Design and Application of Inorganic Nanoparticle Superstructures: Current Status and Future Challenges*, Small 7, 2133 (2011)

Meso Town Halls for Community Input

Boston APS Wed Feb 29 5:45 PM Convention Center 253C

MRS San Francisco Mon Apr 9

ACS Webinar April 24

Chicago middle May

Special Kavli Symposium on Emergent Physics at the Mesoscale
Wednesday, February 29th, 2012 at 2:30 pm (Boston Convention Center)
Session Chair: Kate Kirby (APS)

Speakers with Tentative Titles:

Robert Laughlin M-02-20-02 - Perspectives in Emergent Mesocopic Physics

William Phillips M-02-20-03 - Quantum Information and Mesoscale physics

Angela Belcher M-02-20-04 - Self Assembly on the Mesoscale

William Bialek M-02-20-05 - The Mesoscale Interface between Physics and Biology

George Whitesides M-02-20-06 - Biological Physics on the Mesoscale

Meso Web Page for Background and Input

http://www.meso2012.com

Input wanted!