
Quantum to the Continuum: Opportunities for Mesoscale Science

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What is meso?

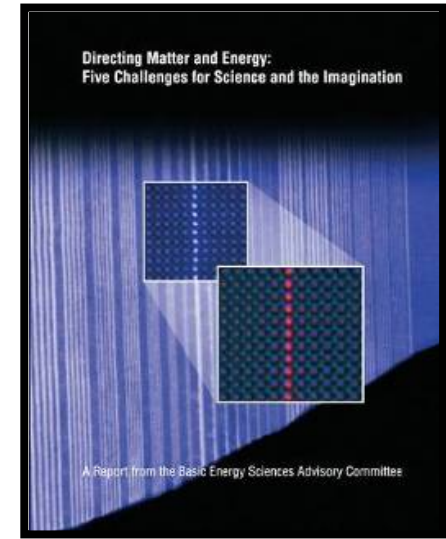
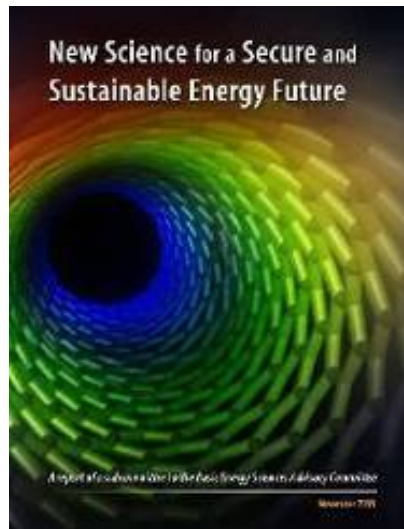
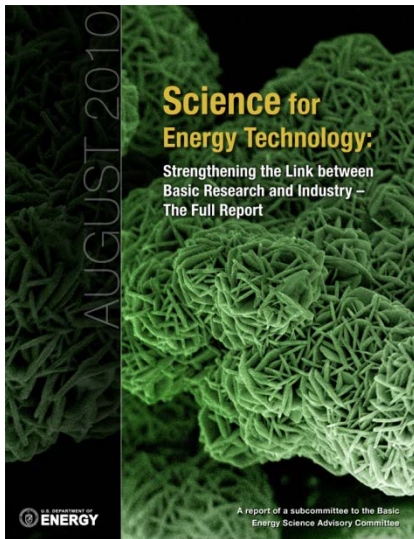
Meso themes

Meso tools



Background

- Why: **the need for innovation**, as articulated in *Science for Energy Technology*
- Why now: **the insights and tools we've gained (and are still gaining)** from nanoscience, as articulated in *New Science for a Secure and Sustainable Energy Future*
- What: build on **basic science challenges**, as articulated in *Directing Matter and Energy: Five Challenges for Science and the Imagination*



What is Meso?

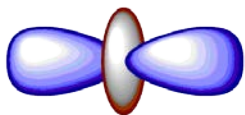


What is Meso?

from the Greek

In between, intermediate, middle

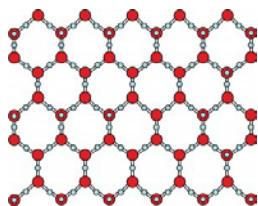
Relative, not absolute



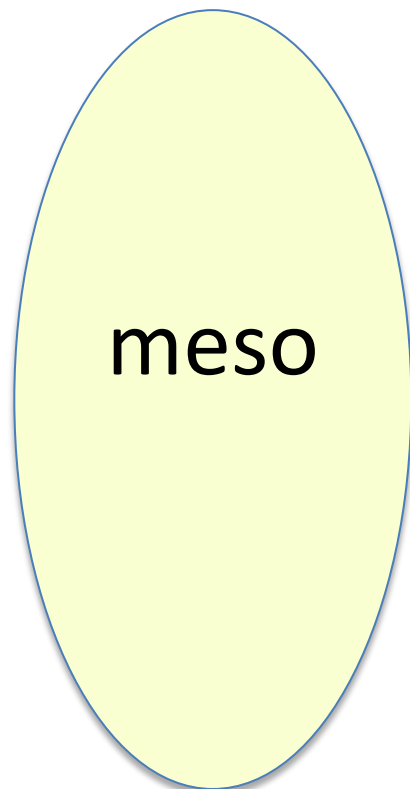
quantum



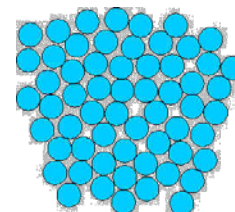
isolated



simple



classical



interacting



complex

Focus on structure, dynamics, and function



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What is Meso? An Opportunity Space

Multiple degrees of freedom interact constructively

Complexity enables new phenomena and functionality

Consilience of systems and architectures

Biology: an inspiration and proof of principle

Biological complexity with inorganic materials

Multiple spatial, temporal and energy scales meet

Quantum meets classical

Top-down meets bottom-up

Multi-scale dynamics essential for functionality

At the meso scale, new organizing principles are needed

Meso embraces emergent as well as reductionist science

What laws govern deterministic assembly?

Key Themes: Quantum to the Continuum

Defect Evolution and Damage Accumulation

Functional Mesoscale Systems

Reactive Transport in Mesoporous Media

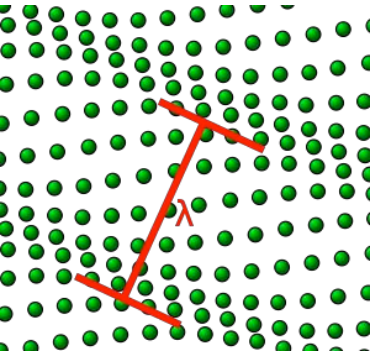
Bio-inspired Assembly and Transduction



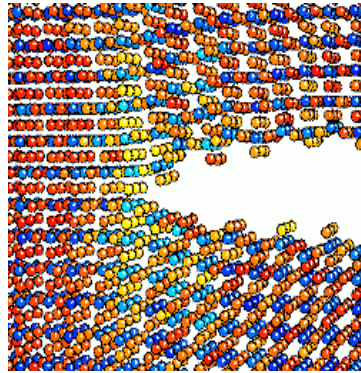
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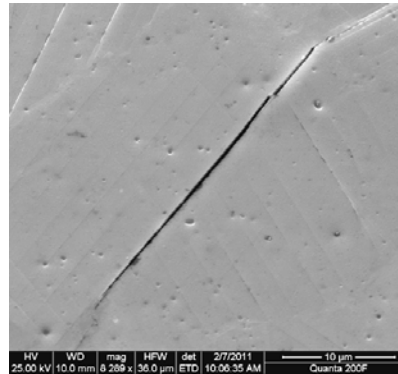
Defect Evolution and Damage Accumulation



Deformation



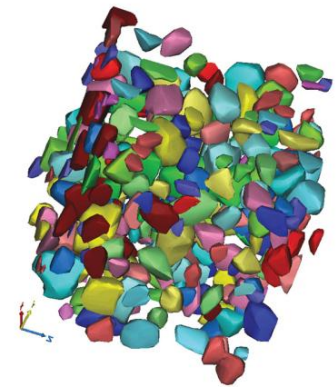
Crack
Initiation



Crack
Propagation



3D Coherent
Imaging



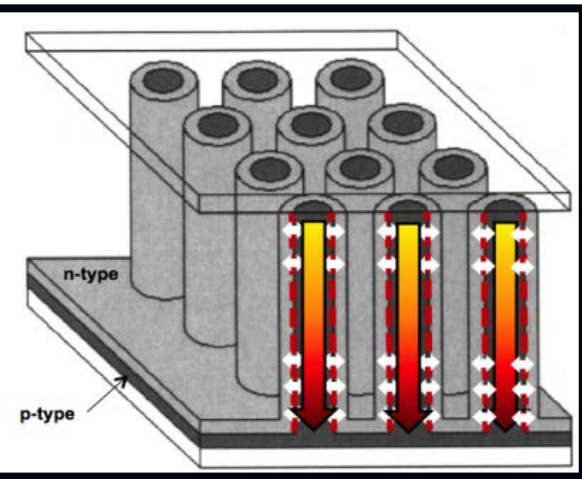
x-ray tomography

Failure



Functional Mesoscale Systems

Solar cell



Phenomena

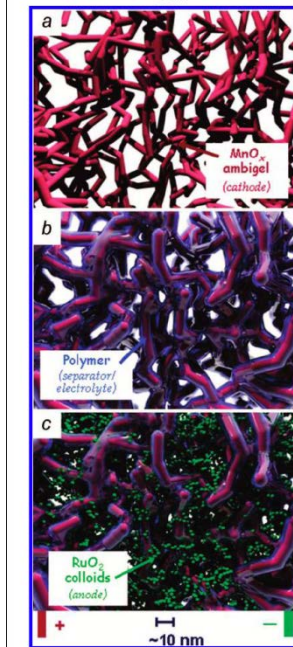
Ionization

Ion insertion/extraction

Electronic / ionic conduction

Volume expansion/contraction

Battery



Meso

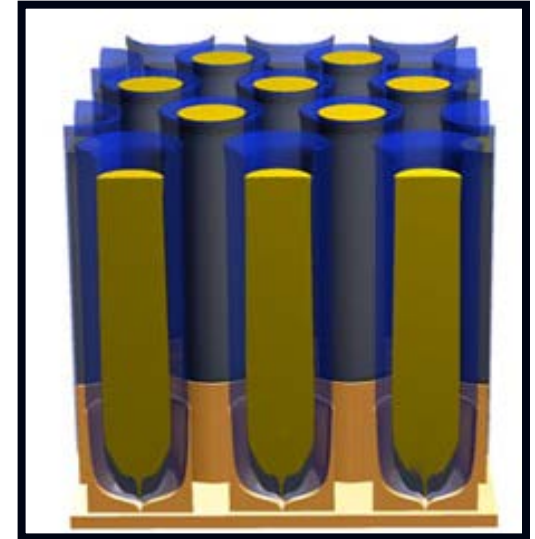
Functionality

Energy storage

Energy delivery

Reversibility on demand

Super capacitor



Degrees of freedom

Electronic

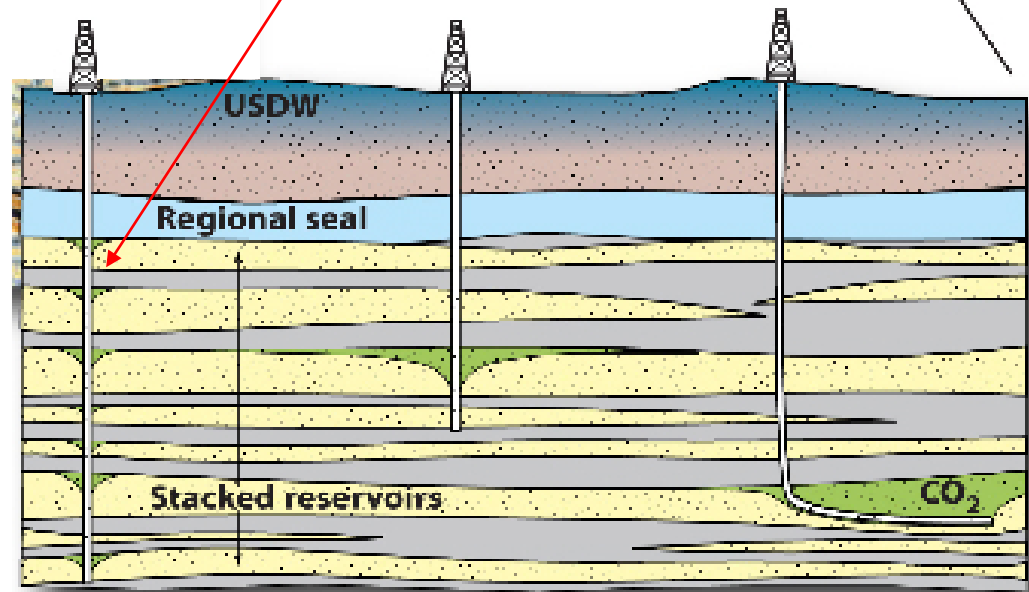
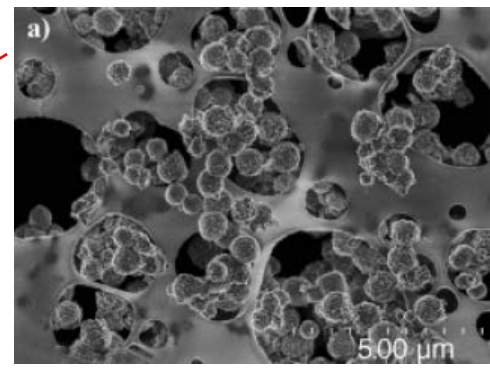
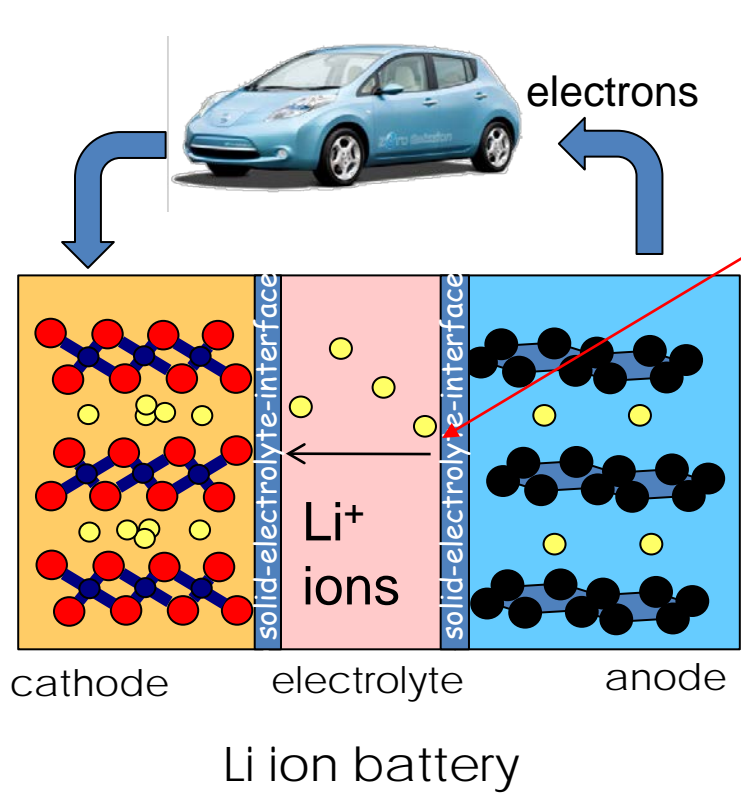
Ionic

Chemical

Mechanical



Reactive Transport in Mesoporous Systems



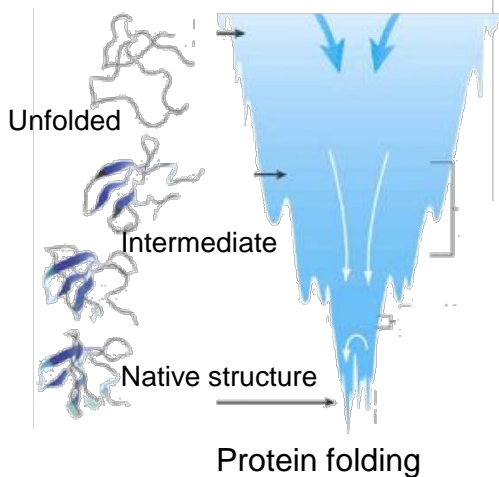
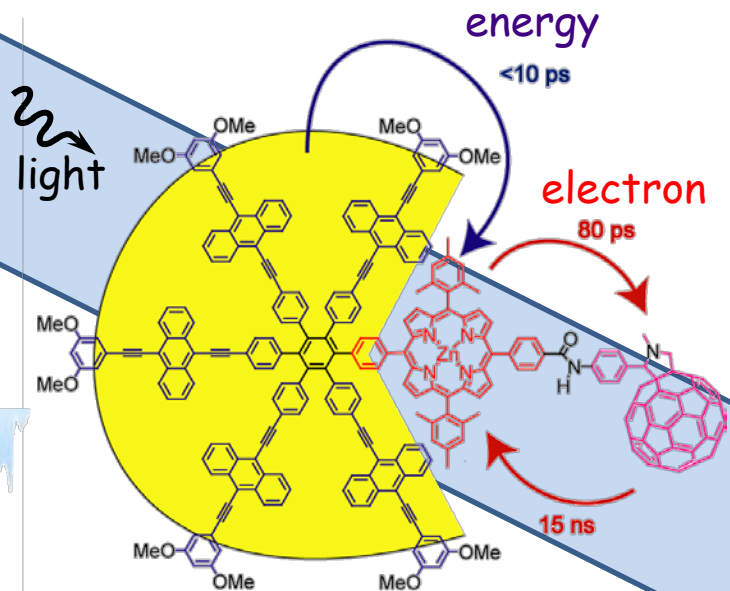
CO_2 sequestration

Bio-inspired Assembly and Transduction

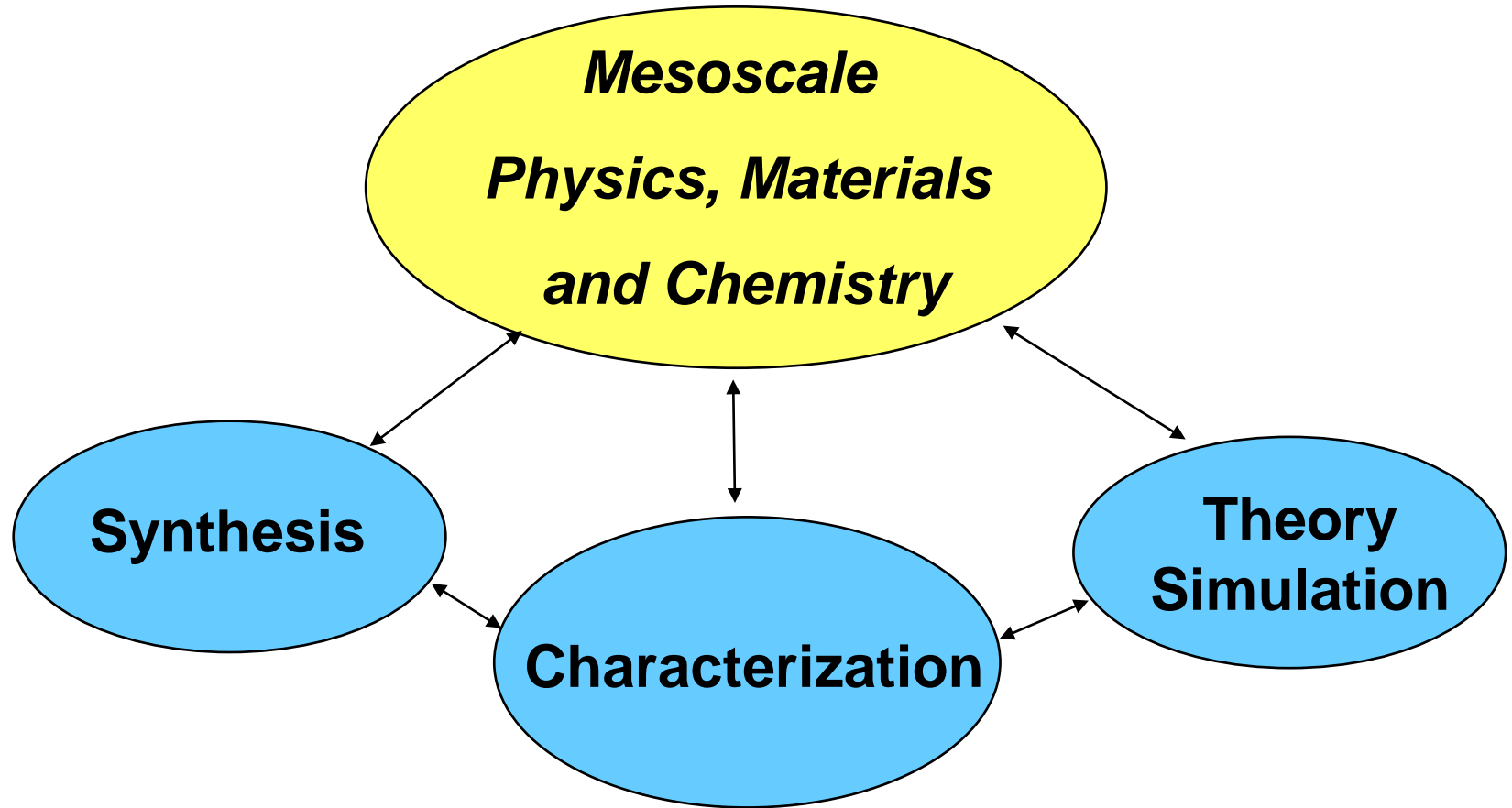
Elements of Assembly

- compositional structural \longrightarrow functional unit
- architectural \longrightarrow connecting functional units
- temporal \longrightarrow connecting sequential steps

many interacting degrees of freedom



Realizing the Meso Opportunity: Tools and Instruments



Mesoscale Tools and Instruments

Synthesis / Assembly

- Directed synthesis of complex inorganic materials
- Multi-step, multi-component assembly processes
- Computational synthesis / assembly

Characterization

- In situ, real time dynamic measurements:
4D materials science
- Multi-modal experiments, e.g. structure + excitation + energy transfer
- Multi-scale energy, time and space

Theory / Simulation

- Far from equilibrium behavior
- Heterogeneous/disordered systems
- Dynamic functionality of composite systems

Cross-cutting Challenges

- Co-design/integration of Synthesis \leftrightarrow Characterization \leftrightarrow Theory/Simulation
- Directed Multi-step, multi-component assembly processes that scale
- Multi-modal simultaneous and sequential measurements
spanning energy, length & time scales
- Predictive theories and simulation of dynamic functionality

Venues for Community Input: Town Halls and Website

APS Boston Wed Feb 29

Marc Kastner and William Barletta (MIT), hosts

ACS San Diego Tues Mar 27

John Hemminger, Douglas Tobias (UCI), hosts

MRS San Francisco Mon Apr 9

Cynthia Friend, Gordon Brown (Stanford/SLAC)
Don DePaolo, Paul Alivisatos (Berkeley/LBNL), hosts

ACS Webinar Thu April 12

John Hemminger, Douglas Tobias (UCI), hosts

Meso2012.com

