70 YEARS OF CREATING TOMORROW

Los Alamos NATIONAL LABORATORY

Opportunities for Mesoscale Science: A MaRIE Perspective

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UNCLASSIFIED

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

NNSA National Nuclear Security Administration

LANL Mission & Vision

Our mission as a DOE national security science laboratory is to develop and apply science, technology, and engineering solutions that

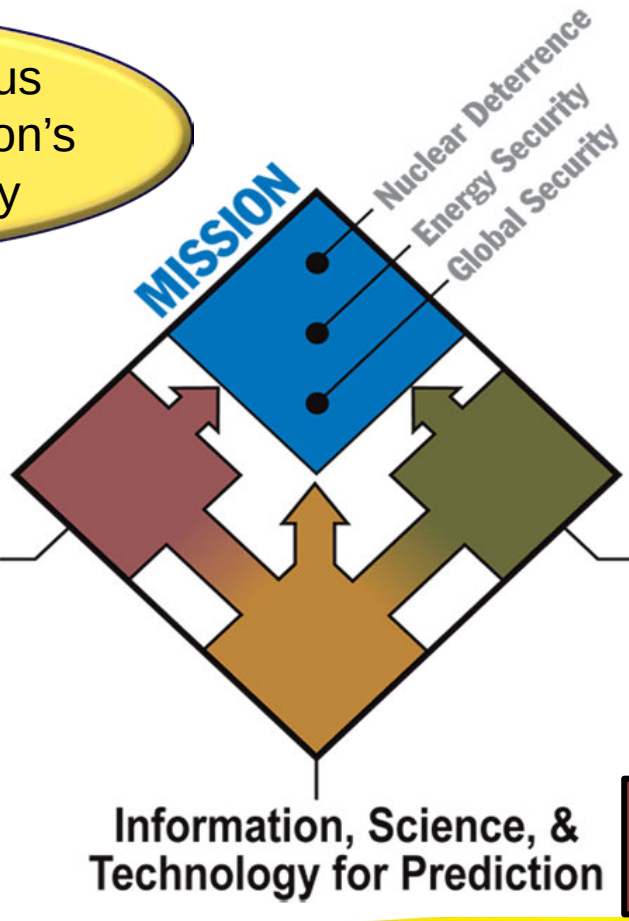
- Ensure the safety, security, and reliability of the US nuclear deterrent
- Protect against the nuclear threat
- Solve Energy Security and other emerging national security challenges

Our vision is to be the premier National Security Science Laboratory

ST&E Capability Pillars provide *cross-cutting capability focus* for our national security missions

National Security Science

Los Alamos is a nexus for advancing the nation's security & prosperity

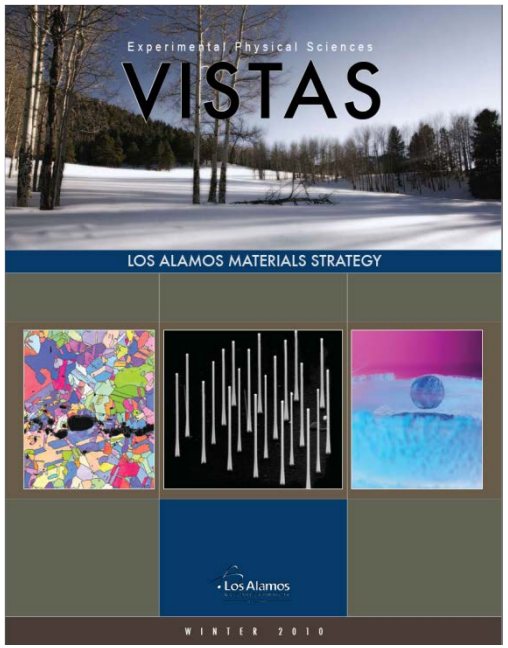


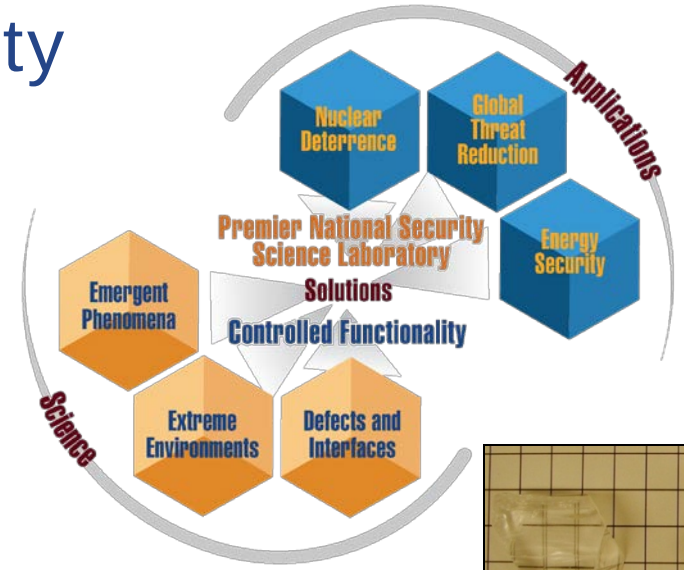
discover signatures, revolutionize measurements, and forward deployment

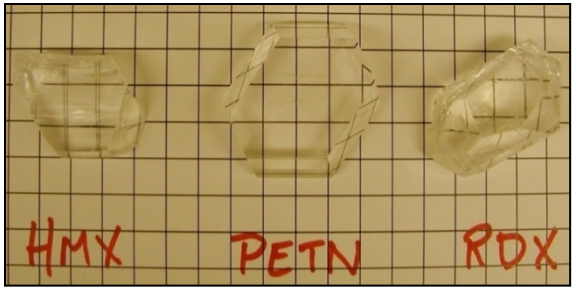
defects and interfaces, extreme environments, and emergent phenomena

data science at scale, computational co-design, and complex networks

Materials Pillar:
Controlled Functionality







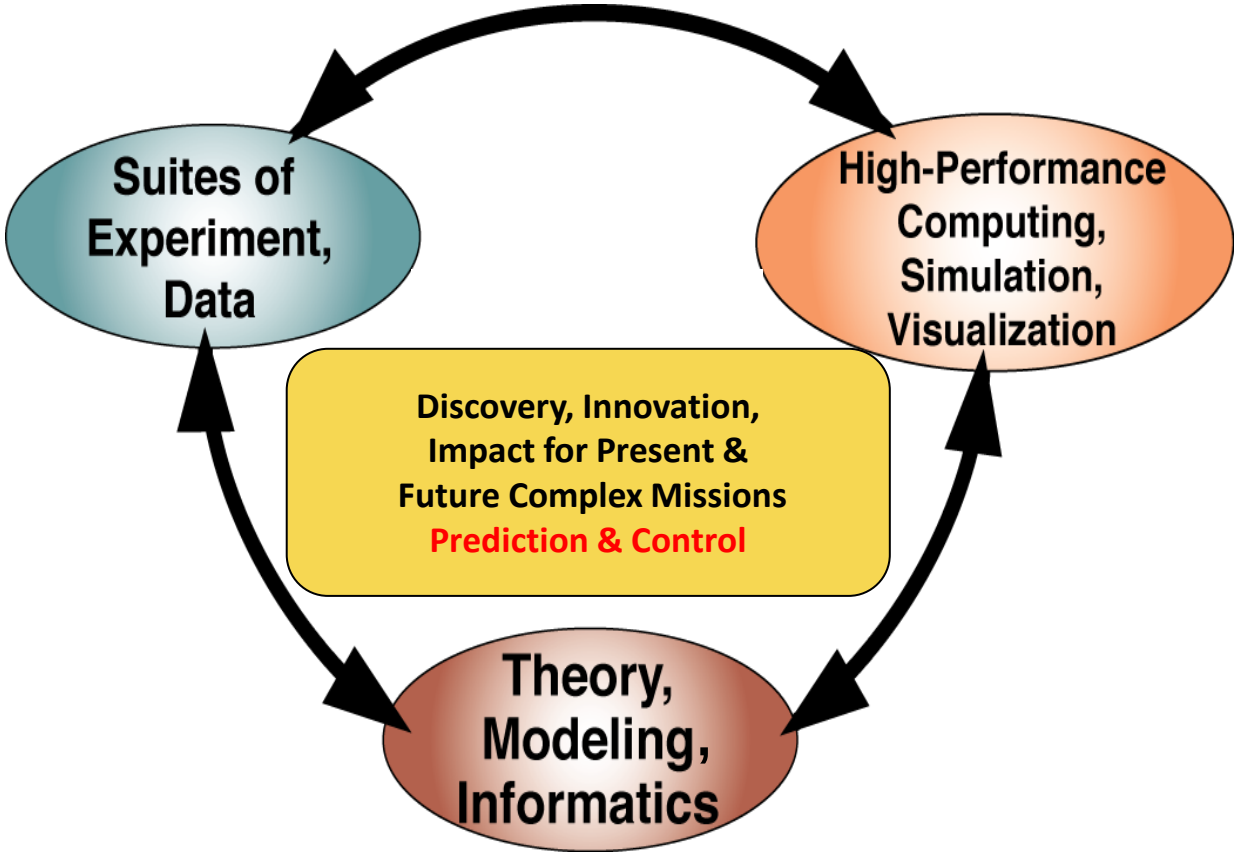
The Materials Strategy advances our vision to develop materials with 'controlled functionality' to provide solutions enabling LANL's missions

STRATEGIC and IMPLEMENTATION PLANS

We predict and control functionality through forefront science and engineering across three themes:

- Defects and Interfaces
- Extreme Environments
- Emergent Phenomena

Co-Design is How We do Our Work



science.energy.gov/bes/news-and-resources/reports/basic-research-needs/

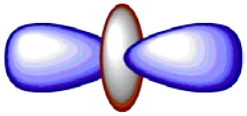
From Quanta to the Continuum: Opportunities for Mesoscale Science

John Sarrao
George Crabtree

Co-chairs
BESAC subcommittee
on Mesoscale Science

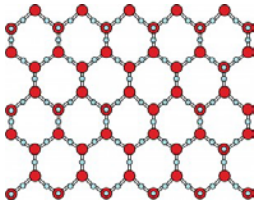
www.meso2012.com/

Meso: Beyond atomic, molecular, and nano



quantum

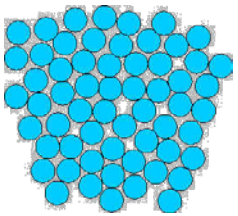
isolated



simple
perfect
homogeneous

meso

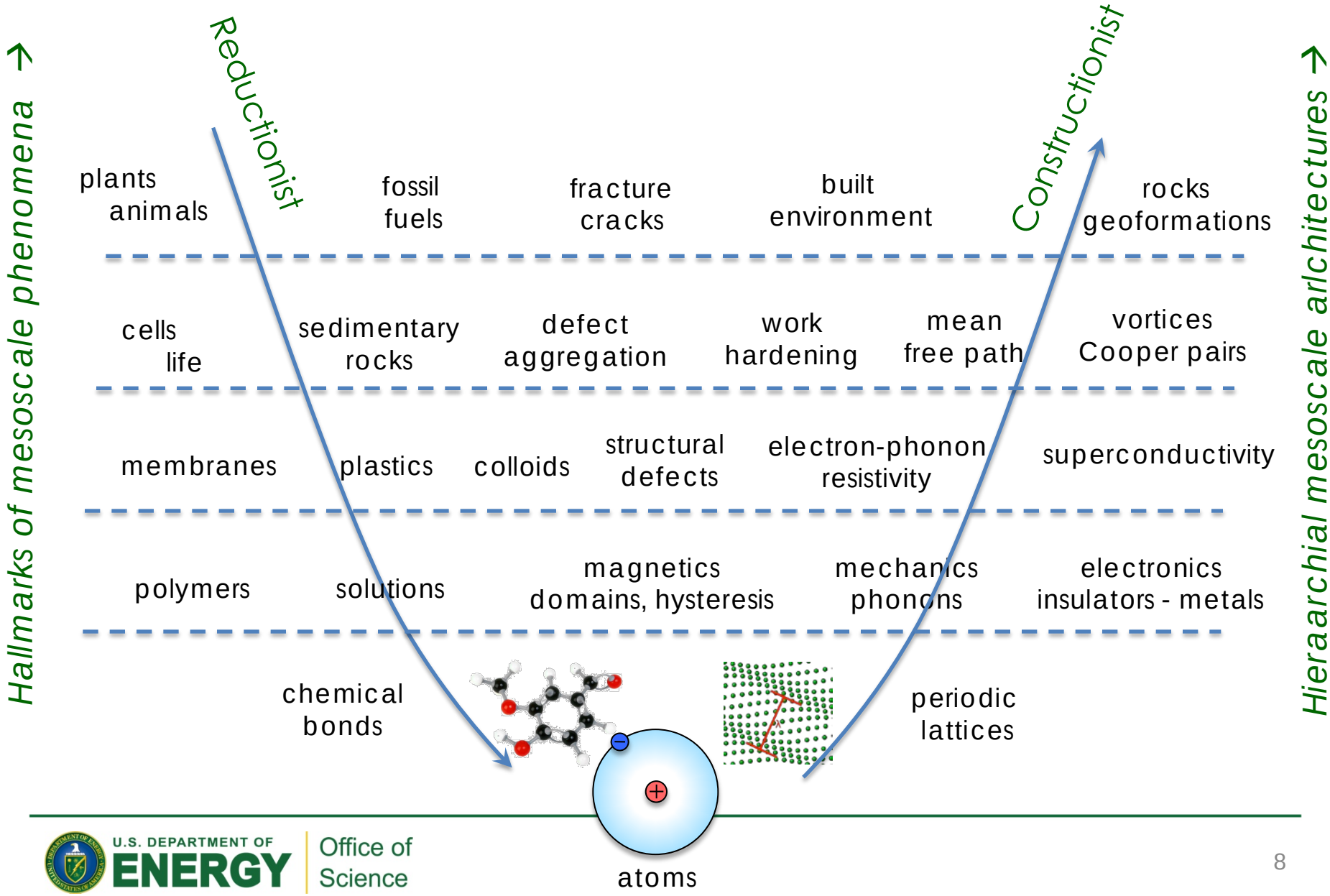
classical



interacting
collective

complex
imperfect
heterogeneous

Meso: a Constructionist Drive from the Bottom Up



Perspective on Mesoscale Science

A new frontier, where quanta meet the continuum:

Six hallmarks of meso phenomena

atomic granularity; energy quantization; collective behavior;

interacting degrees of freedom; defects, fluctuations and statistical variation;
heterogeneity of structure and dynamics

Hierarchy of mesoscale architectures

based on chemical bonds and periodic lattices

Integration of disciplines and specialties

especially computation with synthesis and characterization

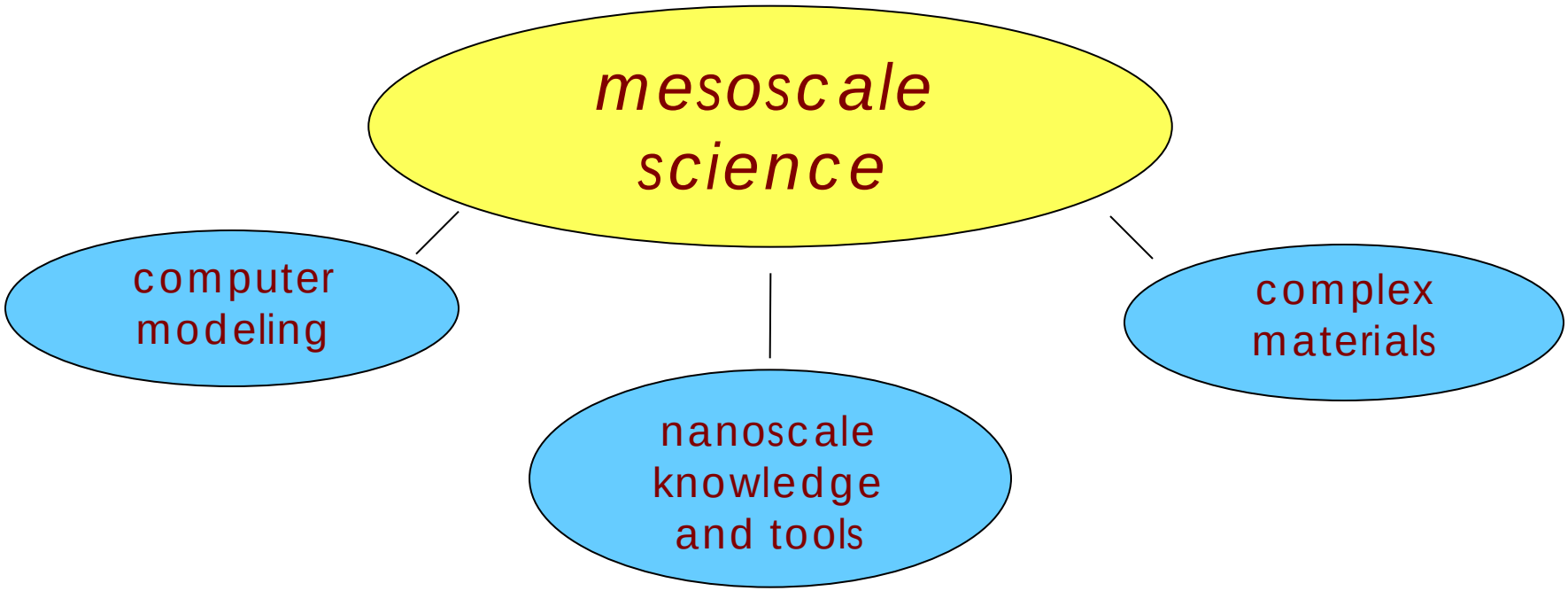
Multimodal tools for in situ spatial and dynamic resolution

Constructionist science from the bottom up

innovative and complex mesocale architectures
new horizon of targeted macroscale behavior, functionality and technology

a discovery laboratory for finding new phenomena
a self-assembly foundry for creating new functional systems
a design engine for new technologies

Why Now?



A solid foundation in nanoscale science

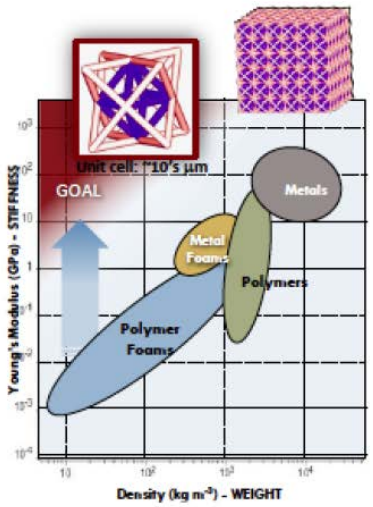
intense sources and scanning probes for ultrafast and ultrasmall characterization

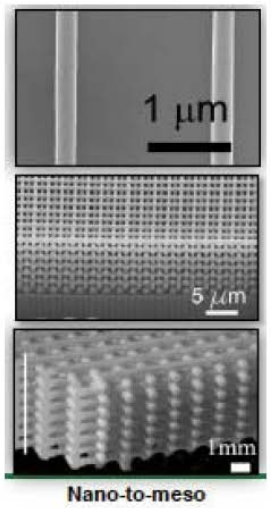
established top down and nascent bottom up synthesis cultures need to be joined

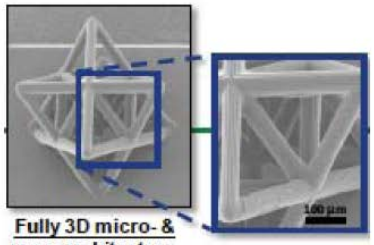
Computer modeling of mesoscale complexity within reach

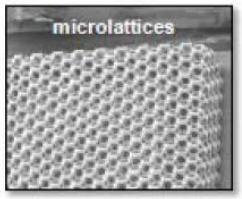
Complex bio-inspired materials a model for constructionist mesoscale science

Creating the materials, structures, and architectures that access the benefits of mesoscale phenomena is a key challenge







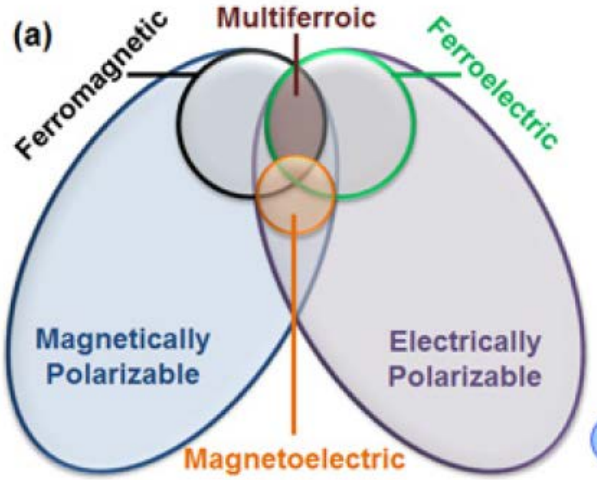


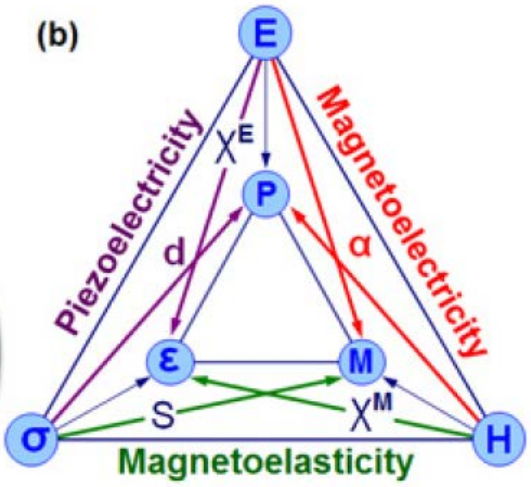
Directed synthesis to create complex materials and controlled interfaces

Assembly processes and pattering strategies

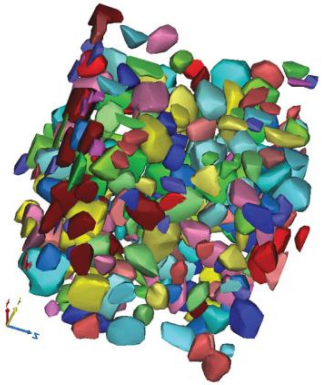
Computational tools for functionality by design

In situ observation and control of synthesis processes





Exciting new sources (e.g., LCLS, NSLS-II, SNS) are available, but need to advance optics, detectors, environments, and data handling



x-ray tomography

New methods to watch multi-d defect evolution & tracking

In situ, in operando measurements

Long duration measurements

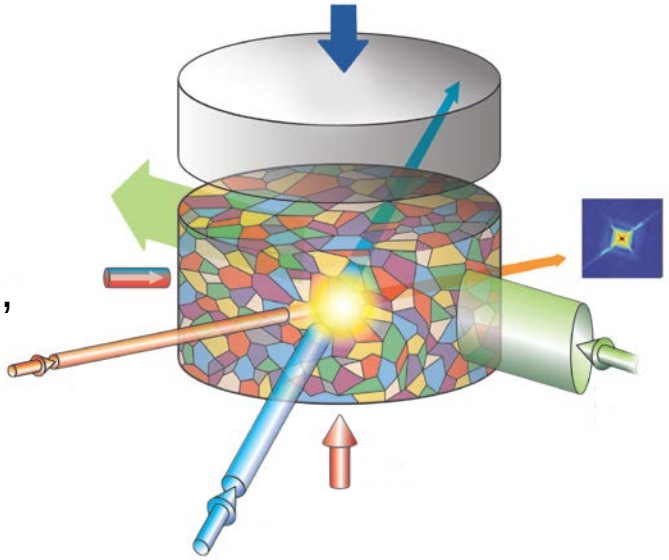
Simultaneous diffraction, imaging and spectroscopy

Dierolf et al, Nature 467, 436 (2010)

3D coherent imaging

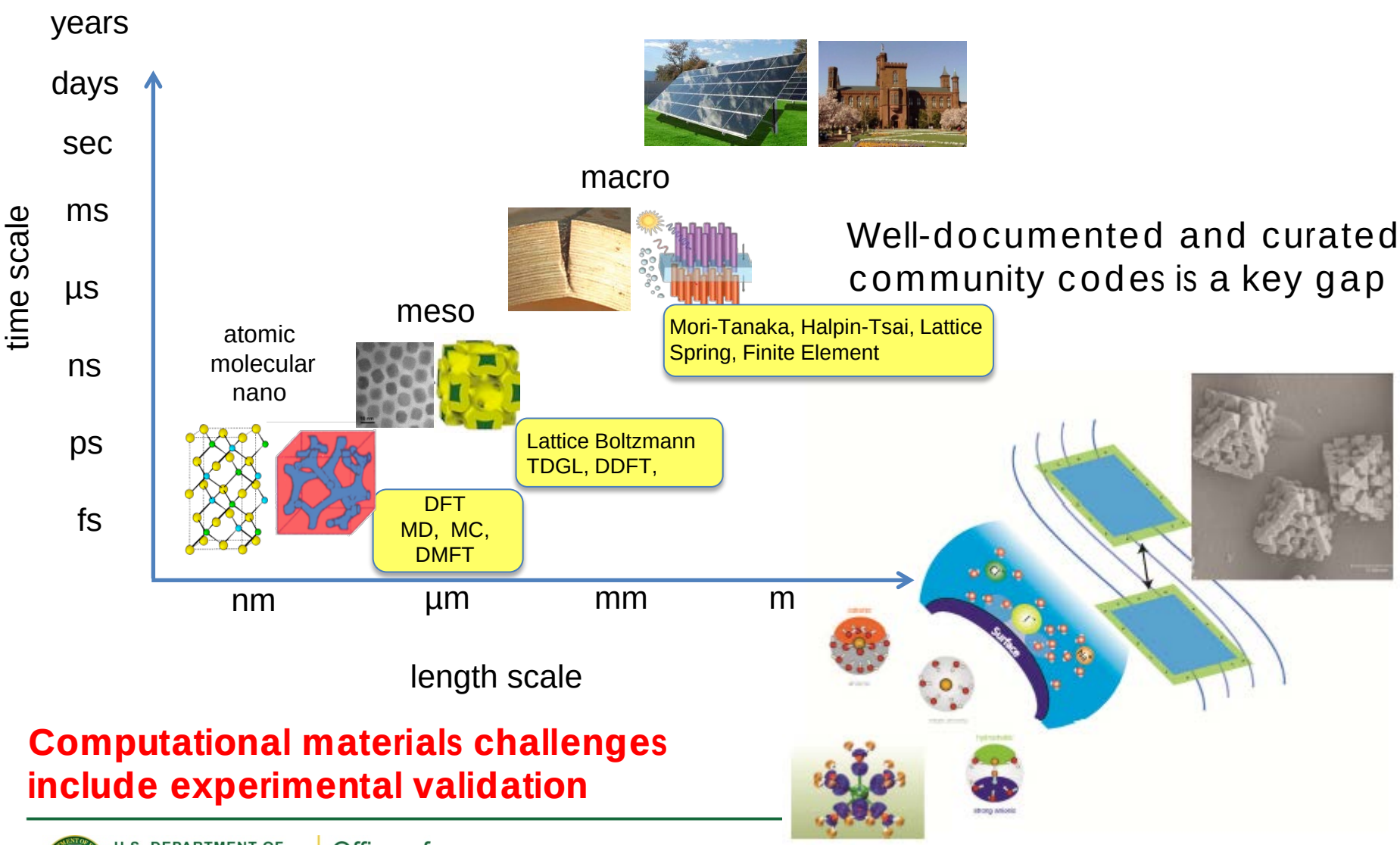
Time-correlated probes of local structure, composition, excitation

Data mining strategies



3 dimensional, in situ, multi-modal measurement

Theory and simulation need to connect models across scales AND incorporate emergent phenomena to realize functionality by design

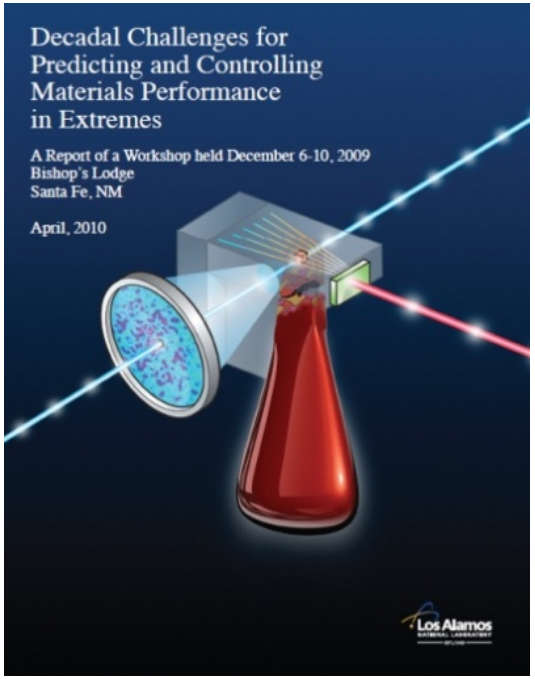


Well-documented and curated community codes is a key gap

Computational materials challenges include experimental validation

Materials research is on the brink of a new era – from observation of performance to control of properties

The confluence of unprecedented experimental capabilities (e.g. 4th generation light sources, controlled synthesis and characterization, …) and simulation advances are providing remarkable insights at length and time scales previously inaccessible



New capabilities will be needed to realize this vision:

In situ, dynamic measurements

simultaneous scattering & imaging

of well-controlled and characterized materials

advanced synthesis and characterization

in extreme environments

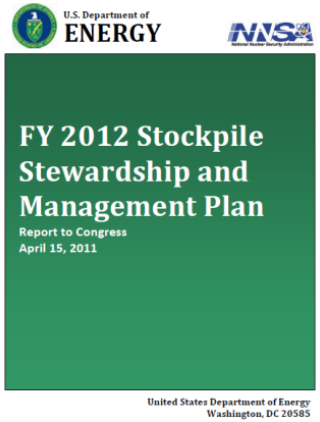
dynamic loading, irradiation

coupled with predictive modeling and simulation

materials design & discovery

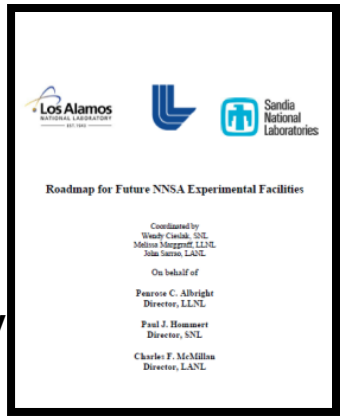
MaRIE, building on LANSCE success, is a key step towards this vision

NNSA Mission Drivers articulate the need for MaRIE 1.0: Dynamic Materials Performance and Process Aware Manufacturing



"Weapons materials aging and replacement material qualification: … there will be an increasing need for more sophistication in predicting their behavior under weapons conditions. In addition, as unavoidable changes in the stockpile occur, models for materials behavior will need to be more closely related to fundamental thermodynamic and physical properties."

"In particular, we believe that filling the gap in our ability to 'predict and control from materials and devices to manufacturing processes' is especially urgent."



Program Drivers	Mission Challenge	Technical Challenge Embodied in MaRIE 1.0 First Experiments
Understand condition of nuclear stockpile	Reduce uncertainty in integrated codes through validated materials models	*Dynamic Materials Performance*
Extend the life of U.S. nuclear warheads	Understand role of aging on hydrodynamic implosion	*Dynamic Materials Performance* *Process Aware Manufacturing*
	Predict performance of manufactured replacements	*Process Aware Manufacturing*
Strengthen the Science, Technology, and Engineering (STE) Base	Understand future needs Expand capability to deal with broader challenges Protect against technological surprise Advance competencies that are the foundation of NNSA mission Invest in technical workforce	*Dynamic Materials Performance* *Process Aware Manufacturing*

We do not presently possess an adequate predictive, process-aware understanding of materials performance

To summarize, by bridging the gap in mesoscale understanding of materials, MaRIE 1.0 will provide three general enhancements to capabilities needed by the stockpile stewardship program:

- **The ability to directly validate material models that transcend scales for certification to supplement the scaling and surrogacy programs already in place,**

- **The ability to develop process aware material models that permit robust development of qualification standards, and**

- **An experimental platform that allows the ongoing development and evaluation of stewardship skills related to material modeling.**

We believe that these capabilities will enhance and complement the otherwise excellent set of scientific tools available to us in the stewardship endeavor.

A suite of fundamental, focused, and integrated experiments is required for success

A short history of MaRIE: Where we've been and where we're going

(2006-2008)

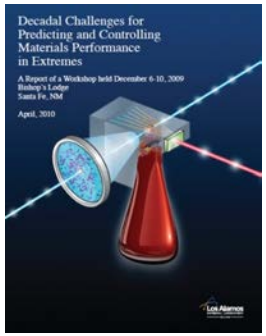
LANS Contract Transition

Concept Definition/Internal Competition

MaRIE selection

Pre-MaRIE

Science Need

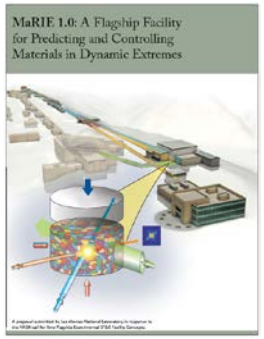


(2009)

Facility Definition

(2010)

Pre-conceptual Proposal



(2012)

Near Term (FY12-FY13) – "MaRIE Proposal":

LANSCE→ Linac Risk Mitigation → MaRIE (including Lujan Center, MTS, …)

MaRIE 1.0: Response to NA-10 "New Facilities" Call (→ CD-0)

Medium Term (FY12 → FY15) – "MaRIE Project":

Facility-specific risk reduction r&d including with partners (e.g., SLAC)

Ongoing –"MaRIE Program":

Doing MaRIE science today, including with partners and at emerging facilities

MaRIE 1.0 is the most mission-relevant subset of MaRIE

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

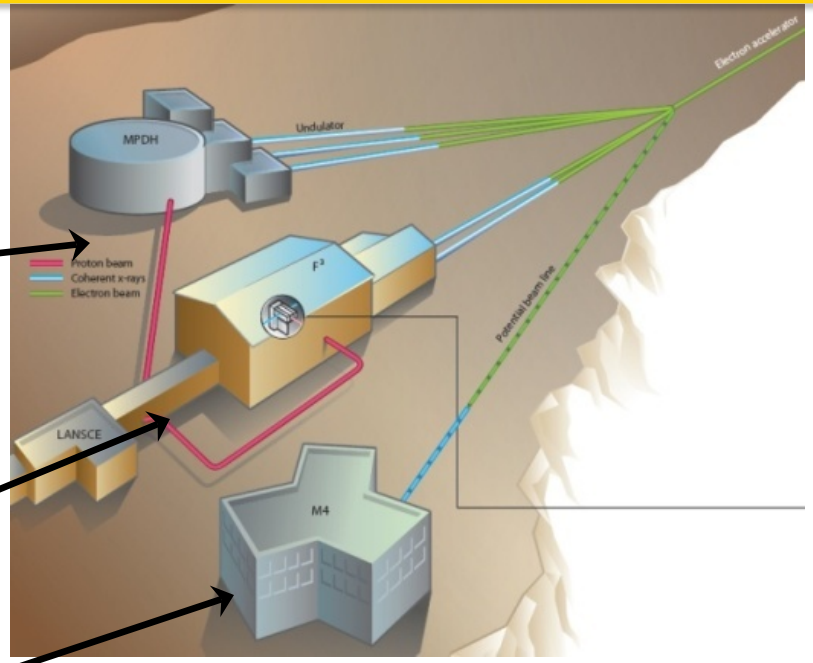
(**MPDH**: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(**F^3**: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(**M4**: Making, Measuring & Modeling Materials Facility)

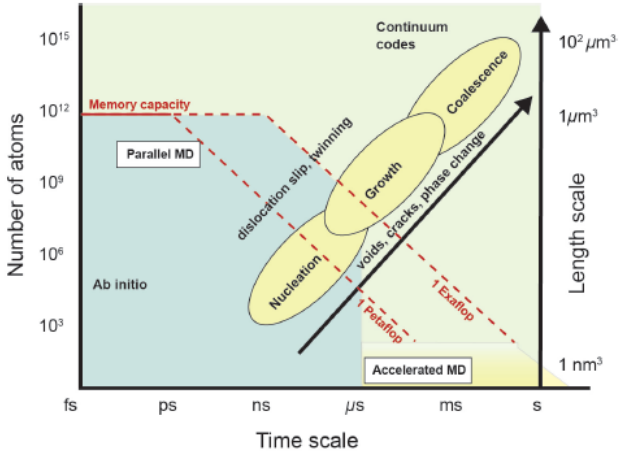


Unique very hard x-ray XFEL

Unique simultaneous photon-proton imaging measurements

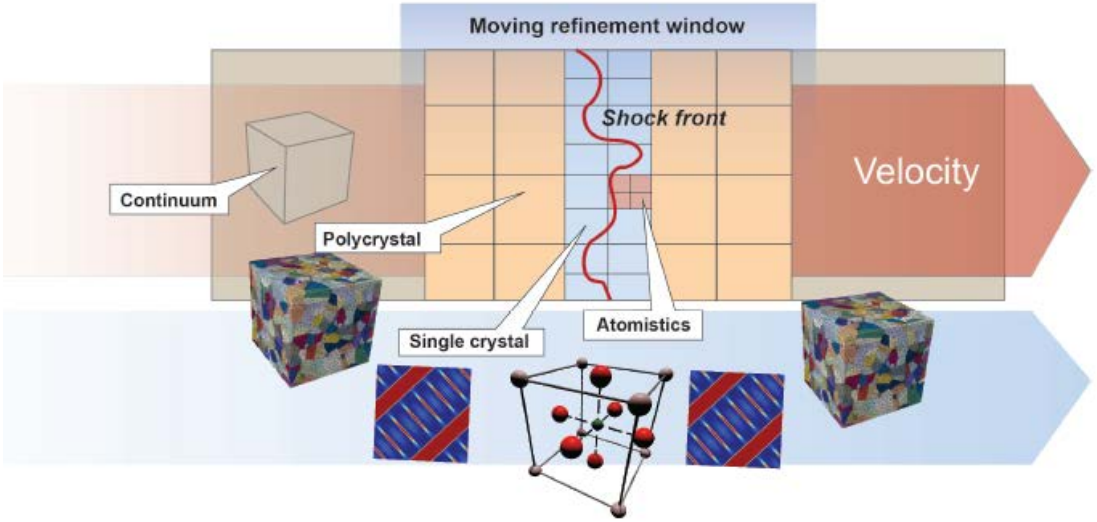
MaRIE will provide unprecedented international user resources

MaRIE 1.0 with LANL's integrated co-design approach will couple multi-scale theory and multi-probe experiment on next-generation computing architectures for future integrated codes



Mesoscale materials phenomena need extreme-scale computing

Variable-resolution models are synergistic with multi-probe, in-situ, transient measurements



The development of MaRIE 1.0-validated models will reduce uncertainty in integrated codes and provide predictive descriptions of newly manufactured materials & components

MaRIE 1.0 will be a national user facility, building on LANSCE infrastructure and leveraging community engagement

LANSCE provides significant site credit and accelerator operations expertise for MaRIE 1.0
-e.g., classified & open experiments on materials of interest (Pu, HE, etc.)

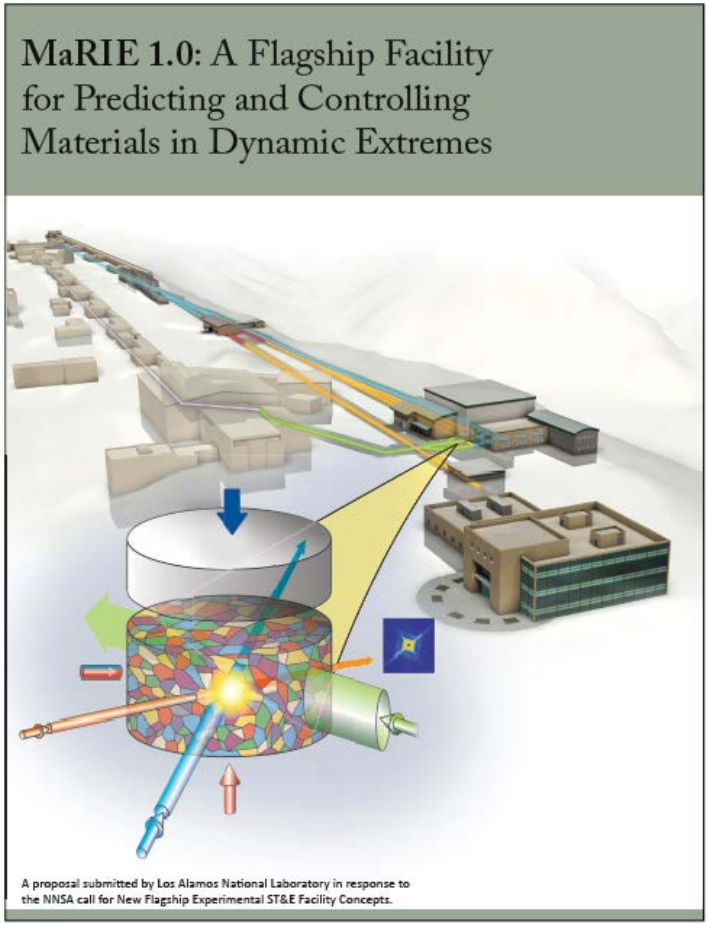
Community workshops provide a snapshot of MaRIE 1.0 user community – **an essential pipeline for future LANL workforce**

Amy Clarke, PECASE
pRad

Kyle Ramos
APS

Richard Sandberg
Cindy Bolme
LCLS

MaRIE 1.0 will enable us to observe and ultimately control how mesoscale materials properties affect performance



A mission need exists for a facility focused on predicting and controlling materials in extreme environments, exploiting *in situ* transient measurements on real materials in relevant dynamic extremes to address key mission challenges.

Achieving controlled functionality at the mesoscale through co-design is the **frontier of materials research**.

MaRIE 1.0 meets this need with a robust preconceptual reference design that is grounded in **community-defined mission and scientific requirements**.

We're doing **"MaRIE science"** now, including with partners and collaborators