SAND2012-5723P

Exceptional service in the national interest

Sandia National Laboratories

Energy, Climate, and Infrastructure Security

Enabling Capabilities Overview

2012

U.S. DEPARTMENT OF ENERGY

NNSA

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Enabling Capabilities

Sandia National Laboratories

Energy, Climate, and Infrastructure Security SMU

Energy Margie Tatro Deputy: Andrew Orrell	Climate Rob Leland Deputy: Marianne Walck	Infrastructure Len Napolitano Deputy: Pablo Garcia	Enabling Capabilities Charles Barbour Deputy: Jerry Simmons
Renewables Juan J. Torres	Atmospheric Monitoring Mark Ivey	Resilient Infrastructure Systems Pablo Garcia	**Discovery Science and Engineering** Jerry Simmons
Nuclear Andrew Orrell	Modeling & Analysis John Mitchiner	Cyber Bob Hutchinson	**ARPA-E** Wahid Hermina
Transportation Bob Carling	Carbon Management John Merson	Electricity & Energy Assurance Rush Robinett	**LDRD** Bob Hwang
Efficiency Jerry Simmons	Water Security Ray Finley	International Assurance Jeff Danneels	**Systems Analysis and Policy** Charles Barbour

Discovery Science and Engineering
Jerry Simmons

Advanced Scientific Computing Research (ASCR)
S. Scott Collis

BES—User Facilities (CINT)
Neal D. Shinn

BES—Materials Science
Jerry A. Simmons

BES—Geosciences
John Merson

BES—Bioscience
Blake Simmons

Fusion Energy Sciences
Larry X. Schneider

Discovery Science and Engineering

Sandia National Laboratories

Deepen fundamental science and engineering competencies in key strategic areas to enable ECIS mission objectives and goals.

Nurture discovery science for fundamental breakthroughs in:

- *Interfacial science*
- *Quantum phenomena*
- *Materials physics*
- *Bioscience*
- *Gas-phase chemistry*
- *Nanosystems*
- *Computational science & math algorithms*

Office of Science
U.S. Department of Energy

Discovery Science and Engineering
Scott Collis

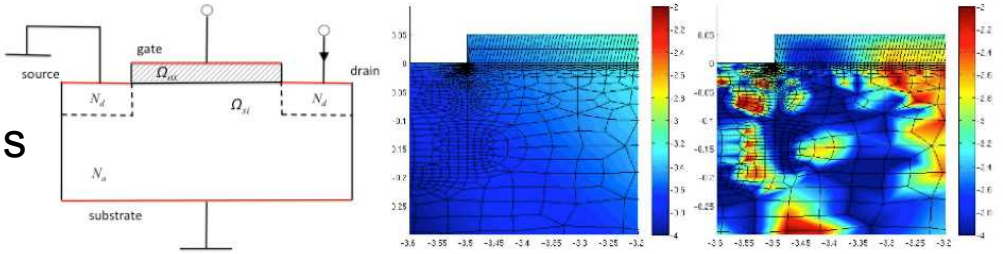
Advanced Scientific Computing Research (ASCR)

Sandia National Laboratories

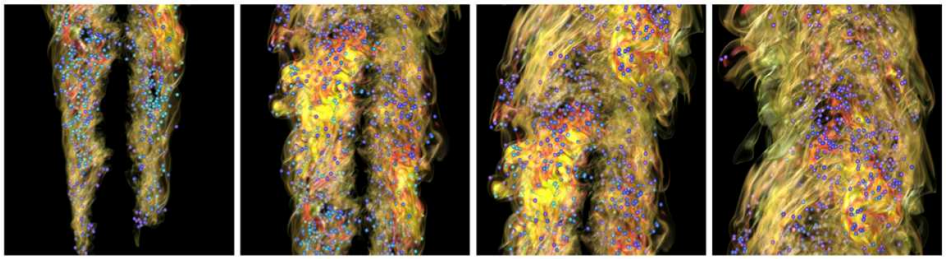
DOE/ASCR Applied Mathematics and Computer Science Research with Application to National-Scale Science

SciDAC Scientific Discovery through Advanced Computing

- **Applied Mathematics Research**
  - Multiscale mathematics
  - Optimization of complex systems
  - Uncertainty quantification
  - Scalable algorithms
- **Computer Science Research**
  - Operating systems
  - Exascale architectures
- **SciDAC3 – Impact to Science**
  - FASTMath: advanced algorithms
  - Quest: uncertainty quantification
  - Climate: atmospheric modeling
- **Exascale Co-Design Centers**
  - Combustion
  - Materials



Rigorous mathematics leads to physical solutions for MOSFET device models (middle) compared to traditional methods that are unstable (right).



Volume and particle visualization from Combustion of methanol

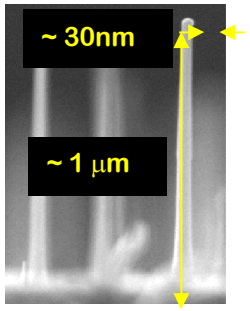
Discovery Science and Engineering
Neal Shinn

BES—User Facilities (CINT)

Scientific User Facility

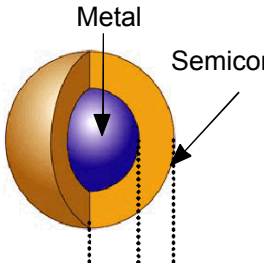
Understanding integration challenges for nanosystems

Synthesis



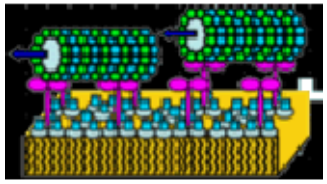
Ge NWs on Si(111)

Heterostructure



Combining ferromagnetic & semiconducting behavior

Assembly



Microtubules + Motor Proteins

Nanosystems

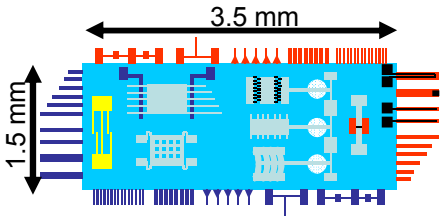
Switchable metamaterials

Nano → **Micro**

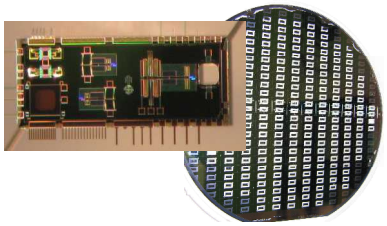
(Length scale)

Nanomechanics and Thermal Transport Discovery Platform™

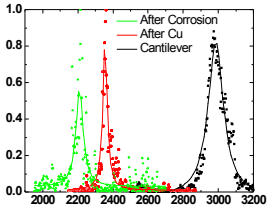
Concept



Platform Realization



Science Results



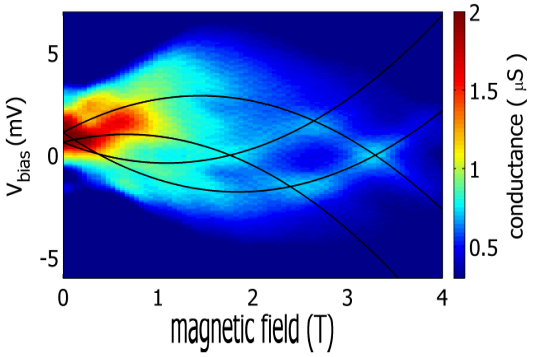
Discovery Science and Engineering
Jerry Simmons

BES--Materials Science

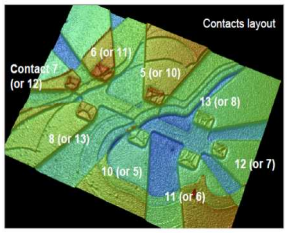
Sandia National Laboratories

Solid State Physics:
Quantum electronics, emergent collective phenomena, semiconductor materials, low-dimensional physics

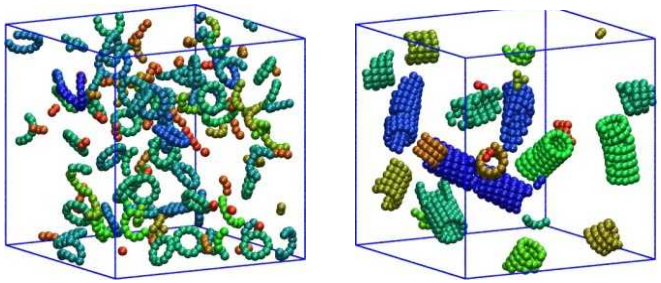
Composite Materials and Interface Science:
Molecular composites, atomic scale self-assembly, interfacial phenomena, mechanics, structure and dynamics



1D – 1D tunneling in double quantum wires

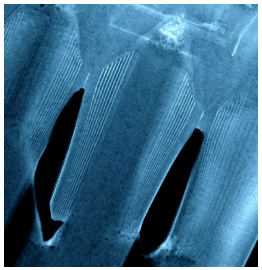


Graphene work draws on both themes

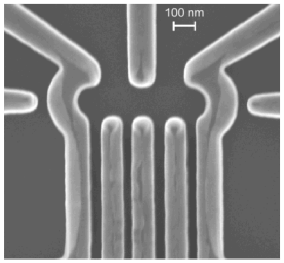


Model for self assembly into microtubules.

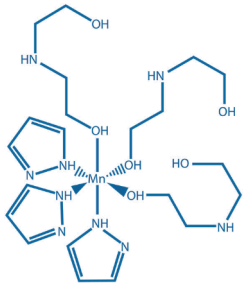
Future Opportunities:



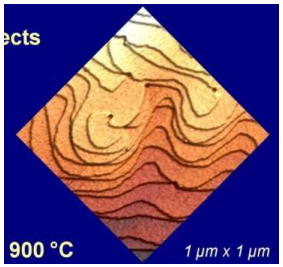
III-nitride core-shell nanowire arrayed solar cells



Solid-State Quantum Information Sciences



New architectures for EE storage



Advanced Epitaxy for Power Electronics

SSLS EFRC
SOLID-STATE LIGHTING SCIENCE ENERGY FRONTIER RESEARCH CENTER

Discovery Science and Engineering
John Merson

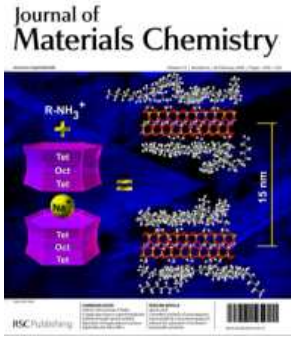
BES--Geoscience

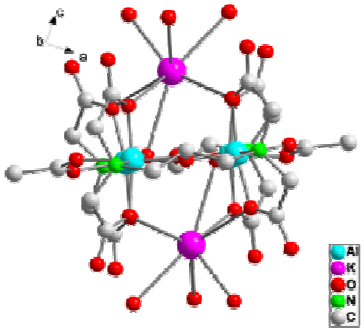
Sandia National Laboratories

Intersection Between the Earth & Engineered Environments

...through research and development in geosciences and sub-surface technologies

Geochemistry: *The Nature Of The Mineral-water Interface*

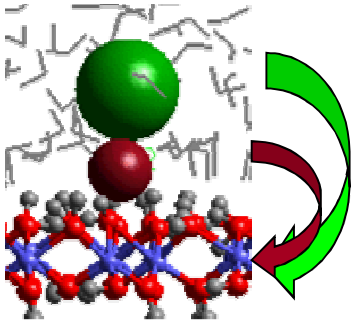




Aluminum cluster showing cation (K^+) association

Anions
Cl^- SO_4^{2-}
SeO_3^{2-}

Metals
Sr^{2+} Pb^{2+}
Hg^{2+}



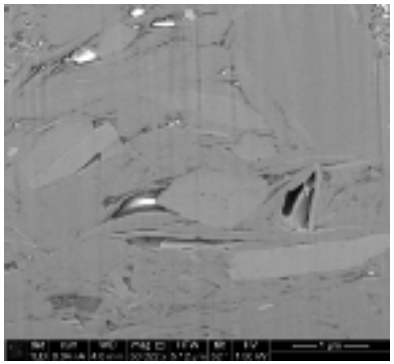
SFG
MM

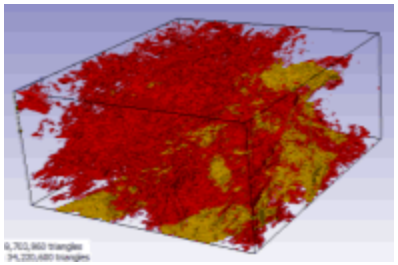
XAS
MM

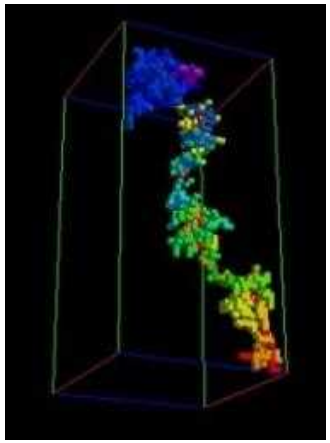
Goethite (FeOOH)

Geomechanics: *Non-Darcian Flow, Imaging and Coupled Constitutive Behavior of Heterogeneous Deforming of Porous Media*

3D Pore Networks and Topology







3D invasion percolation model of a displacing liquid invading pores under capillary pressure. Color indicates relative order of pore-filling (Sandia PERC++ software)

Discovery Science and Engineering
Larry Schneider

Fusion Energy Science

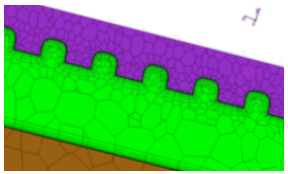
Sandia National Laboratories

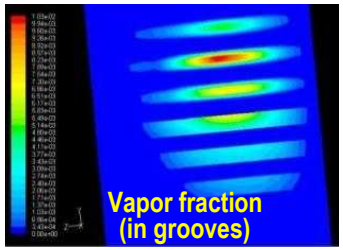
Design, Develop and Test Plasma Facing Components (PFC) & Fundamentals for Inertial Confined Fusion

PFC design & development; modeling, high heat flux tests, joining, fabrication
Plasma edge, plasma wall interactions, tritium retention and permeation
Novel plasma probes – designed and deployed

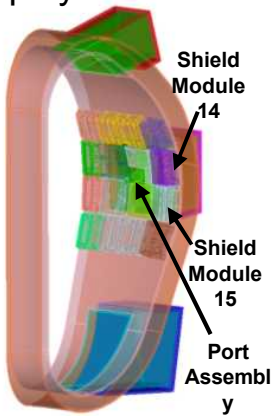
Thermal-hydraulic analysis

Coolant flow and heat transfer reference calculations for ITER.

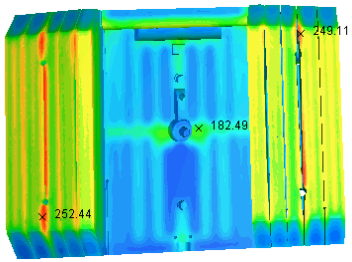




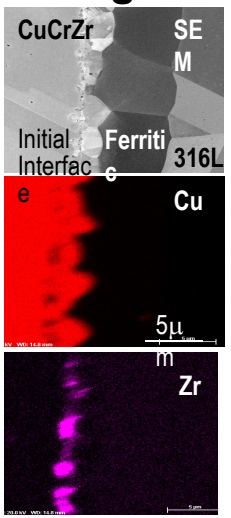
Hypervaportron model (FLUENT) of ITER first wall

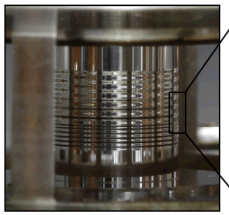


Thermal & stress analyses

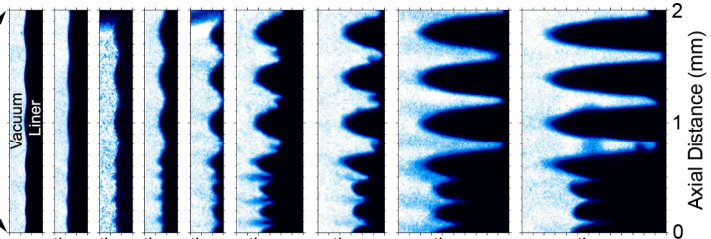


Joining R&D





Pre-test optical photo of perturbed Al liner target



Fundamental Instability Measurements in Magnetically Driven Z-Pinch Liner Implosions: Precision radiography measurements of the growth of the magneto-Rayleigh-Taylor instability that can disrupt magnetically-driven liner target implosions.

ARPA-E
Wahid Hermina

ARPA-E

Sandia National Laboratories

Accelerate industry development of transformational energy technologies through ARPA-E.

Engage with ARPA-E program managers and small businesses to accelerate transformative energy solutions into the market place: develop relationships, collaborations, and exploit Sandia's capability strengths.

- ARPA-E Energy Innovation Summit – develop relationships & collaborations
- Power Electronics Reliability Workshop – determine Sandia's brand
- Continued FOA submissions – as lead and support institution

Current Projects:

GENI: Agile Direct Grid Connect Medium Voltage 4.8-13.8 kV Power Converter for PV Applications Utilizing Advanced Wide Band Gap Devices

ADEPT: Improved Power System Operations Using Advanced Stochastic Optimization

ARRA: Silicase Weathering

Improved Power System Operations Using Advanced Stochastic Optimization(GENI): Sandia, is collaborating with Iowa State University, the University of California at Davis, Alstom Grid, and ISO New England to create a probability-based decision-making software for grid market management systems that can account for the increased uncertainty while retaining overall grid reliability and market stability.

LDRD
Bob Hwang

Laboratory-Directed Research and Development

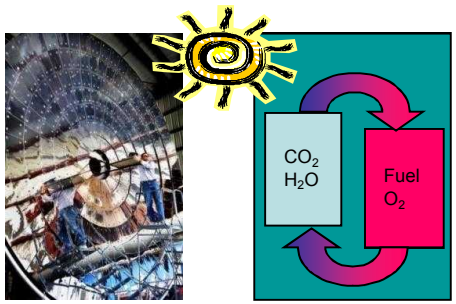
Sandia National Laboratories

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Develop and support SMU-needed capabilities through targeted Laboratory-Directed Research & Development (LDRD) projects.

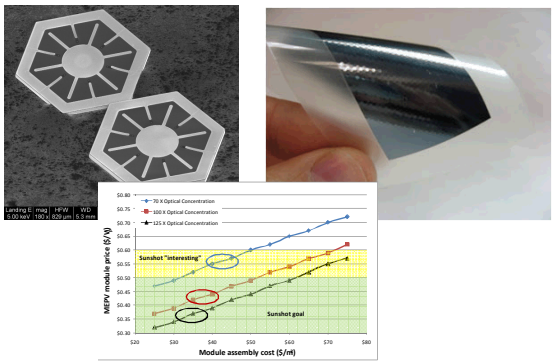
Sunshine to Petrol

Sunlight + CO_2 + H_2O → Fuel + O_2



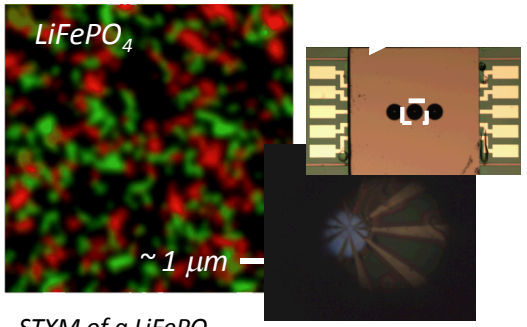
Microscale Enabled Photovoltaics

Enhanced performance from smaller cells and 3-D integration



The Science of Battery Degradation

Create a world-leading battery degradation research team



STXM of a $LiFePO_4$ electrode showing surprising bimodal lithiation.

Optical image looking through the cell

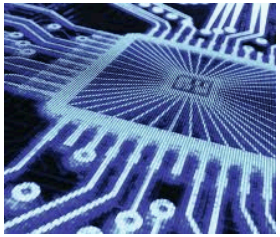
Systems Analysis and Policy
Charles Barbour

Systems Analysis and Policy

Sandia National Laboratories

Creating Enduring Competency and Establishing Leadership in Cybersecurity Analysis —*Susanna Gordon*

- Use knowledge gained from VTCs to develop a proposed method for prioritizing cybersecurity investments in CIKR
- Bring together Sandians from different communities to review methodology and propose improvements



System Impacts of CO_2 Reuse, Reduction, and Storage —*Patrick V. Brady, Peter H. Kobos, and Paul E. Mariner*

- Predict advances in CO_2 management technologies (direct = e.g. sequestration, reuse; indirect = e.g. oxyfuels combustion)
- Assess likely market penetration
- Identify enabling research

ECIS Systems Study: Optimization and Uncertainty Quantification for Atmospheric Sensing and Measurement Systems, with a focus on the Arctic —*Mark Ivey*

- Identify capabilities and critical gaps to address priorities for technology, data, and modeling needs for the scientific and DOD communities.
- Survey potentially high-payoff sources of information.

Robust Energy Policy Analysis (Richard Craft)

Enabling Capabilities Program Challenges

- SC Early Career proposals – need a new approach
- Push to develop a systems analysis capability base that differentiates Sandia from its competition
- Utilize differentiating systems analysis capability to inform policy decision makers at national and state levels
- Building a relationship with ARPA-E that sees SNL as a resource to leverage

Enabling Capabilities questions for EAB

What elements of an energy policy make it robust to political changes (in the nation and globally), and how should SNL support and influence the national debate to achieve a robust US energy policy?

How best should an NNSA Lab that touts itself as an Engineering Lab engage the DOE Office of Science to grow business opportunities?