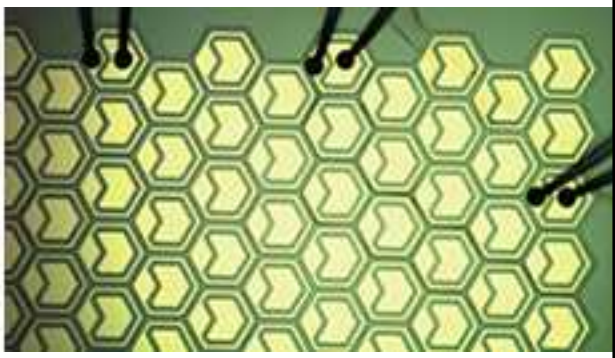
SAND2017-11639PE

Twitter: @SandiaEnergy

Website: energy.sandia.gov





Materials Science and Engineering Programs at Sandia National Laboratories: Ensuring Global Security and Securing our Energy Future

Christian Mailhiot

Sandia National Laboratories -- Livermore, CA 94550

Extreme Crystals Weekend Workshop

University of Nevada, Las Vegas

October 22, 2017

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. SAND2016-0090 PE

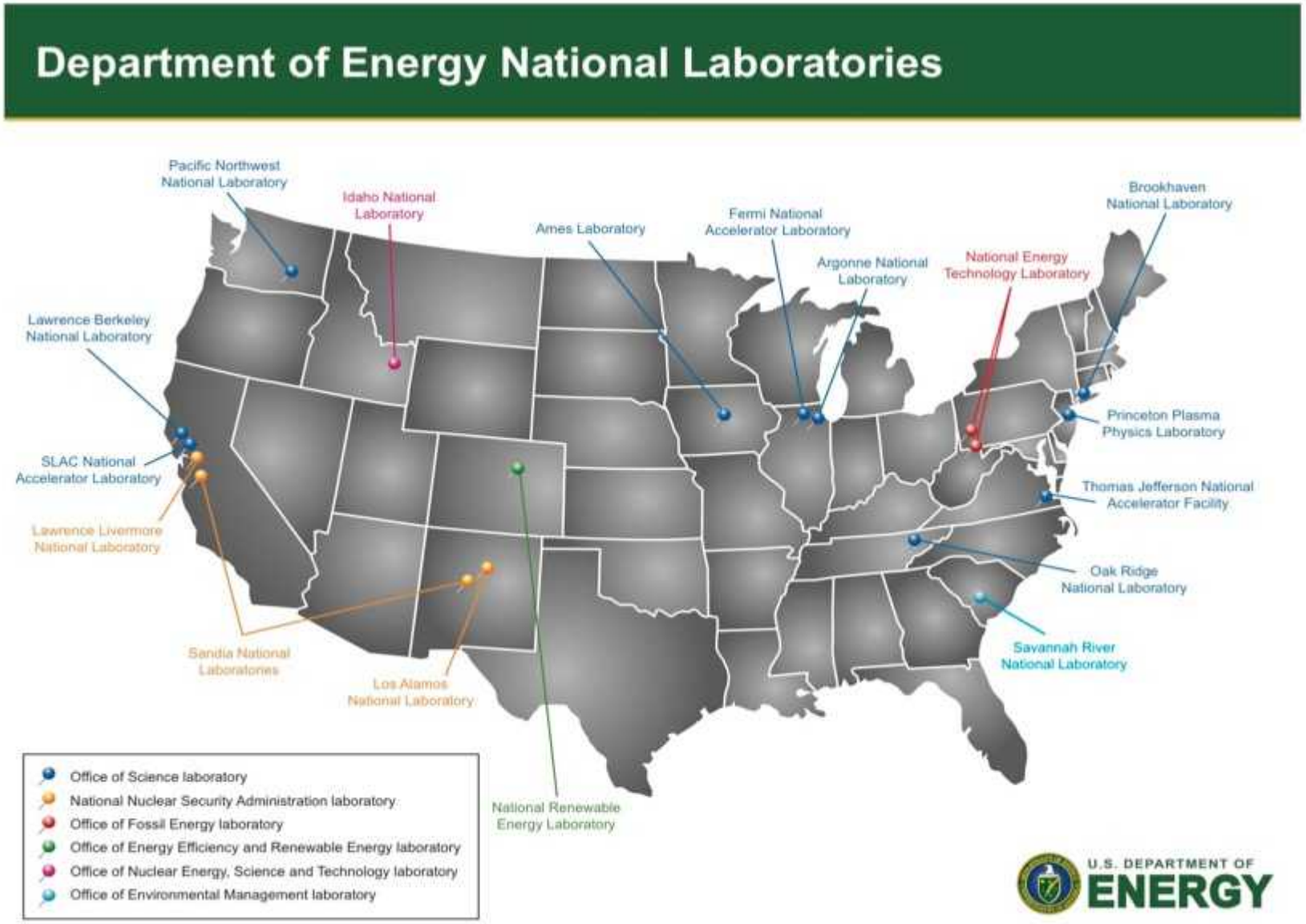
Outline

- Overview of Sandia National Laboratories:
  - Mission
  - Scientific capabilities and core competencies
  - Research infrastructure

- Materials science opportunities at Sandia:
  - Materials in extreme environments
  - Materials for non-conventional computing
  - Quantum materials
  - Materials for energy
  - Advanced manufacturing

Students/postdocs program at Sandia National Laboratories:
http://www.sandia.gov/careers/students_postdocs/

The DOE national laboratories support the agency's broad missions in national security, energy and environment, and discovery science



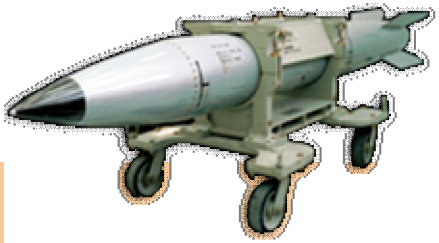
Sandia's mission work supports the nation's global security challenges

1950s	1960s	1970s	1980s	1990s	2000s	2010s
NW production engineering & manufacturing engineering	Development engineering Vietnam conflict	Multiprogram laboratory Energy crisis	Missile defense work Cold War	Post–Cold War transition Stockpile stewardship	Expanded national security role post 9/11	LEPs New START Evolving national security challenges

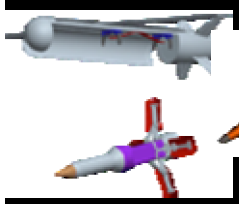
Courtesy of M. Valley, Center 1800, Sandia National Laboratories

Sandia's Mission Foundations

Mission driven innovation enabling mission area success



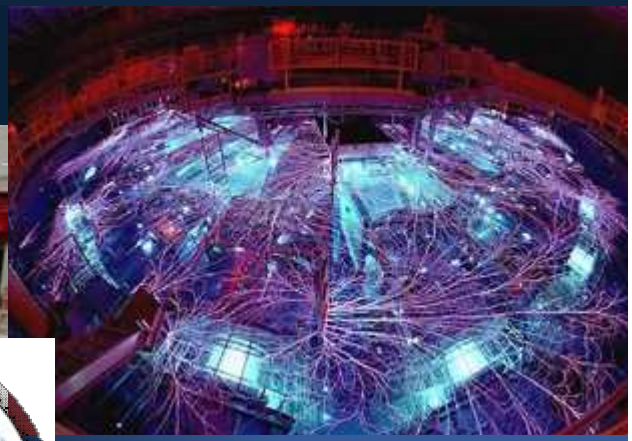
Nuclear Weapons | Energy and Climate | International, Homeland, and Nuclear Security | Defense Systems and Assessments



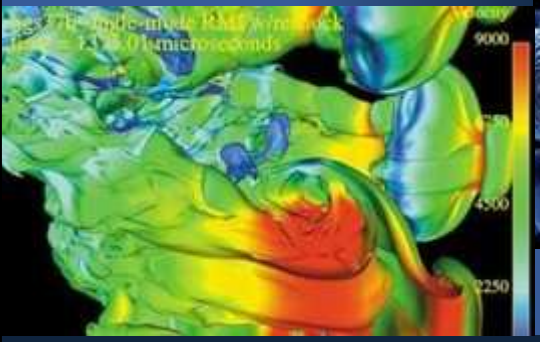
Courtesy of M. Valley, Center 1800, Sandia National Laboratories

Sandia Research Foundations enable responsiveness to mission needs

Computing & Information Sciences

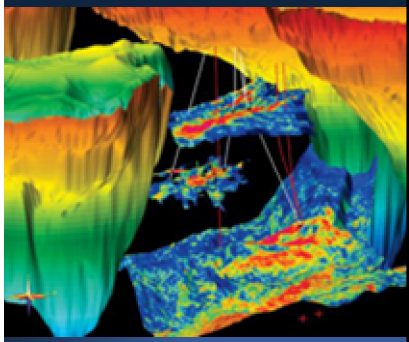


Radiation Effects & High Energy Density Science



Engineering Sciences

Bioscience

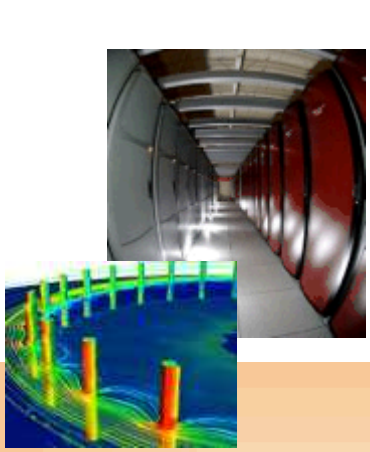


Geoscience

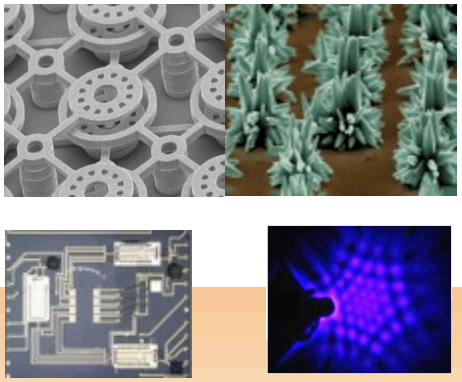
Courtesy of J. Nelson, Sandia National Laboratories

Research disciplines underpin advanced capabilities

Strong research foundations play a pivotal role in Sandia's mission delivery



High Performance Computing

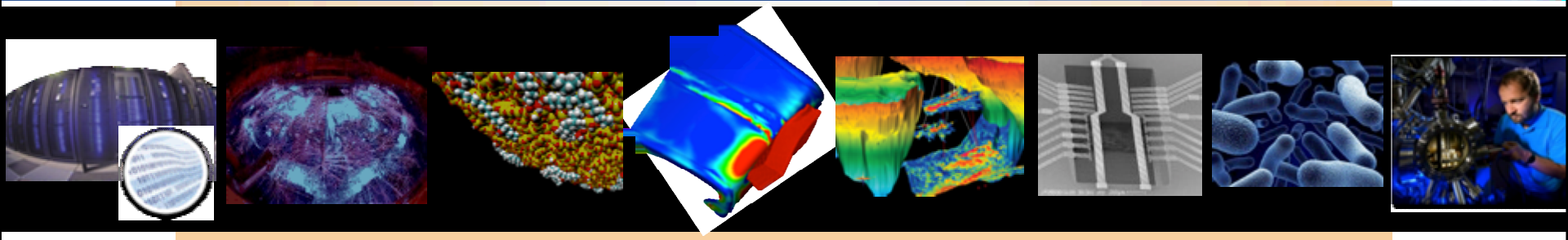


Nanotechnologies & Microsystems

Extreme Environments

Large Scale Testing

Computing & Information Sciences	Radiation Effects & High Energy Density Science	Materials Science	Engineering Sciences	Geoscience	Nanodevices & Microsystems	Bioscience	New Ideas



Courtesy of M. Valley, Center 1800, Sandia National Laboratories

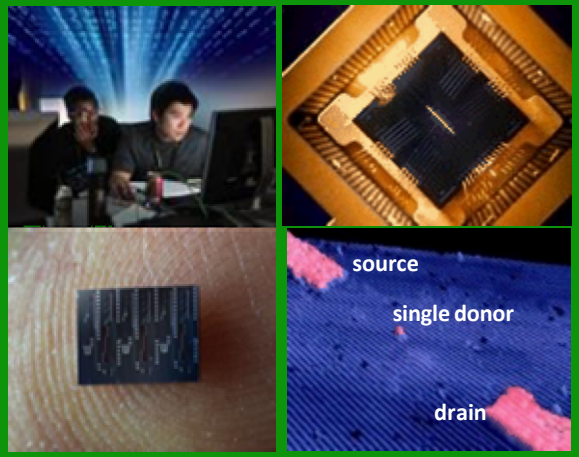
Materials Sciences, Nanodevices, Microsystems Research

"Combine theory, synthesis and characterization to achieve world-leading discovery science"

"Develop the critical and differentiating technical capabilities that will be needed in the future to support our national security missions"

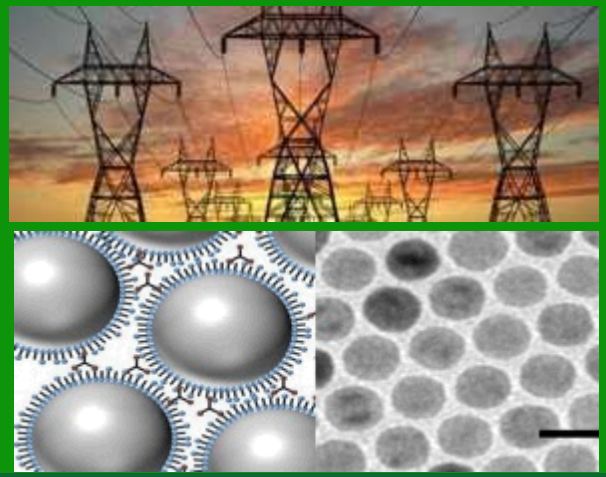
"Discover new phenomena at the nanoscale and microscale; and create or prove new concepts, devices, components, subsystems, and systems."

Cyber and Secure Systems



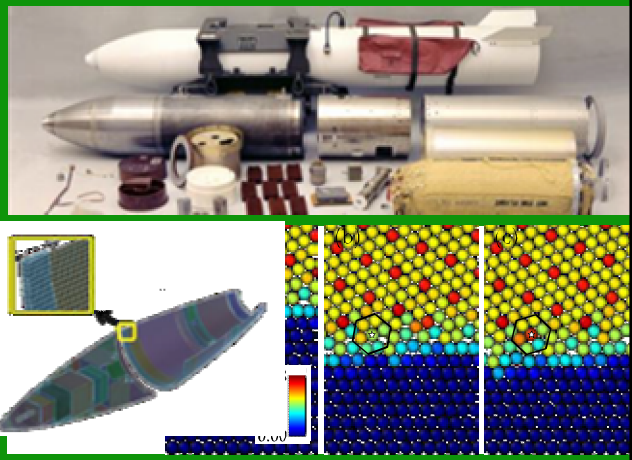
Semiconductors and Quantum Materials

Energy & Climate



Materials Interfaces

National Security



Structural Materials

Courtesy of J. Nelson, Sandia National Laboratories

Leadership-class materials science capabilities and user facilities at Sandia/NM

Microsystems and Engineering Science Applications (MESA)

- 60+ years as DOE/NNSA mission lead in electronics
- Silicon and III-V Materials

Advanced Materials Laboratory (AML)

- Unique materials synthesis efforts

Center for Integrated Nanotechnologies (CINT)

- DOE BES-SUF NSRC
- Celebrating 10th Anniversary
- Focus on Integration of Nanoscience and Technology

Ion Beam Laboratory (IBL)

- Radiation-effects in materials

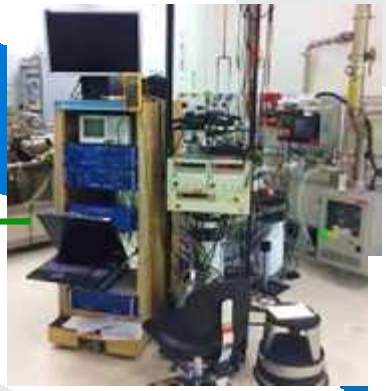
Courtesy of J. Nelson, Sandia National Laboratories

Sandia materials sciences capabilities are available to the research community through the CINT User Program

Single atom dopant incorporation into Si and Si/Ge systems

only such capability in the US

Atomic Precision Lithography



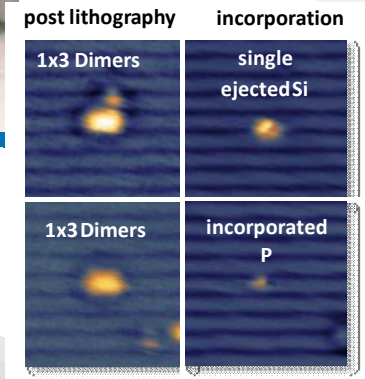
MOCVD and MBE reactors for AlGaInN and AlGaInAsPSb Materials

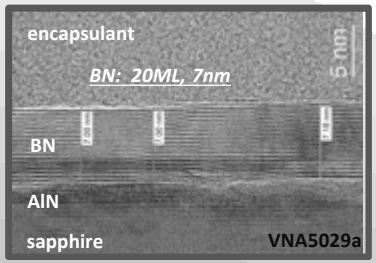
etch pit density < 100 cm^{-2}

Al /sapphire

σ_{RMS} = 0.39 nm

10 μm x 10 μm





Home-built single-wafer hBN MOCVD system capable of operating at ~1600°C

Capabilities descriptions at cint.lanl.gov

Courtesy of J. Nelson, Sandia National Laboratories

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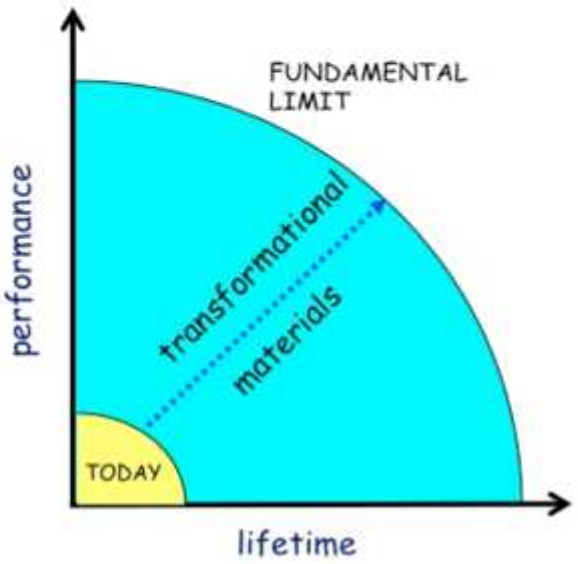
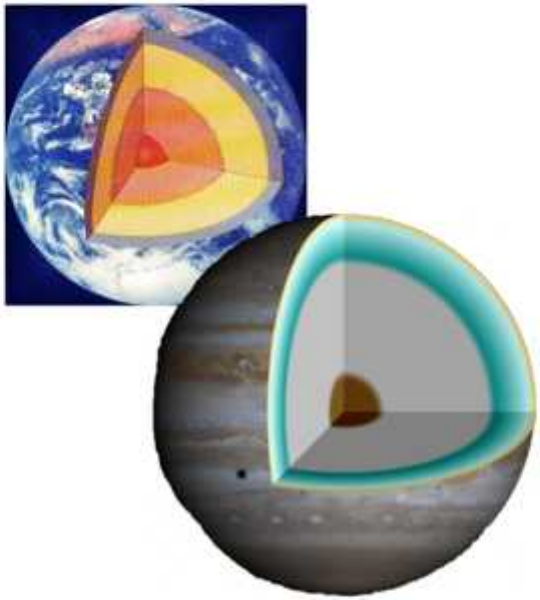
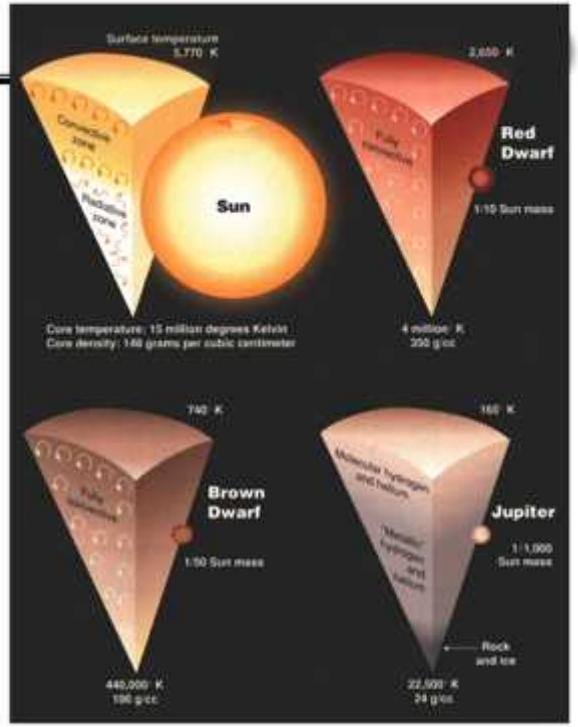
  - Advanced manufacturing

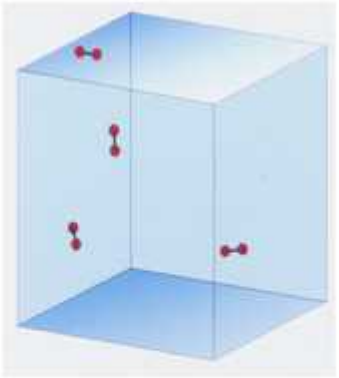
Student program at Sandia National Laboratories:

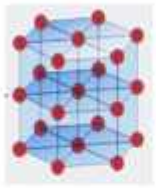
Studies of extreme environments have opened up a new world of materials behavior







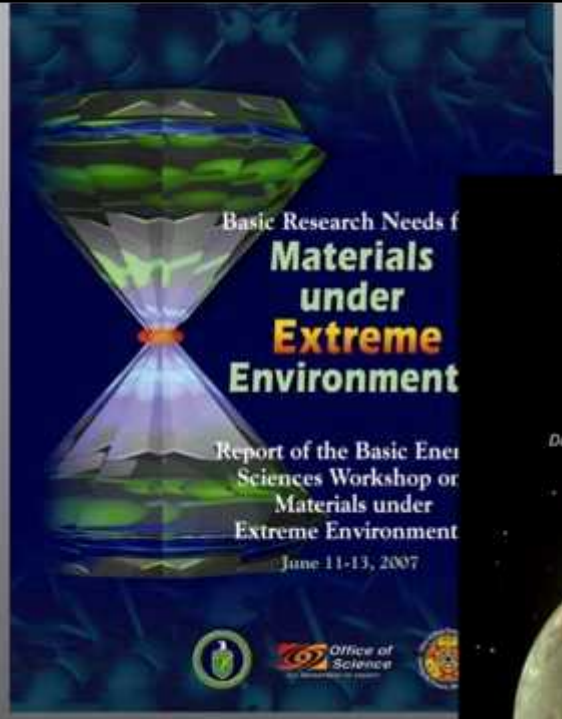




$$\textit{ATOMIC PRESSURES} \quad \frac{e^2}{2a_0{}^4} = 147 \text{ Mbar}$$

- *Materials Science*
- *Physics*
- *Chemistry*
- *Geoscience*
- *Planetology*
- *Biology*

Courtesy of R. Hemley, Carnegie Institution of Washington



This effort builds on a series of reports from previous workshops

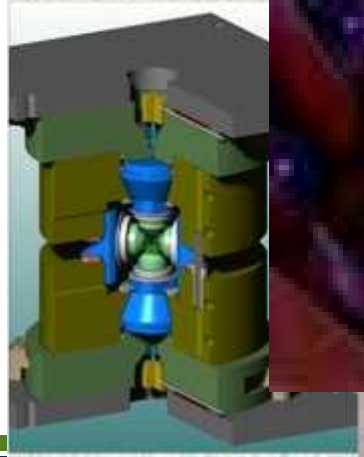
Courtesy of R. Hemley, Carnegie Institution of Washington

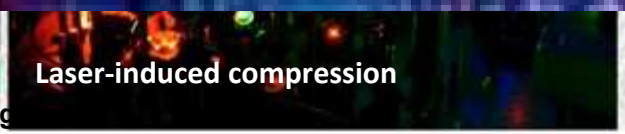
Experimental high-pressure platforms:
Static and dynamic compression

Diamond anvil ce

Large-volu

ndia



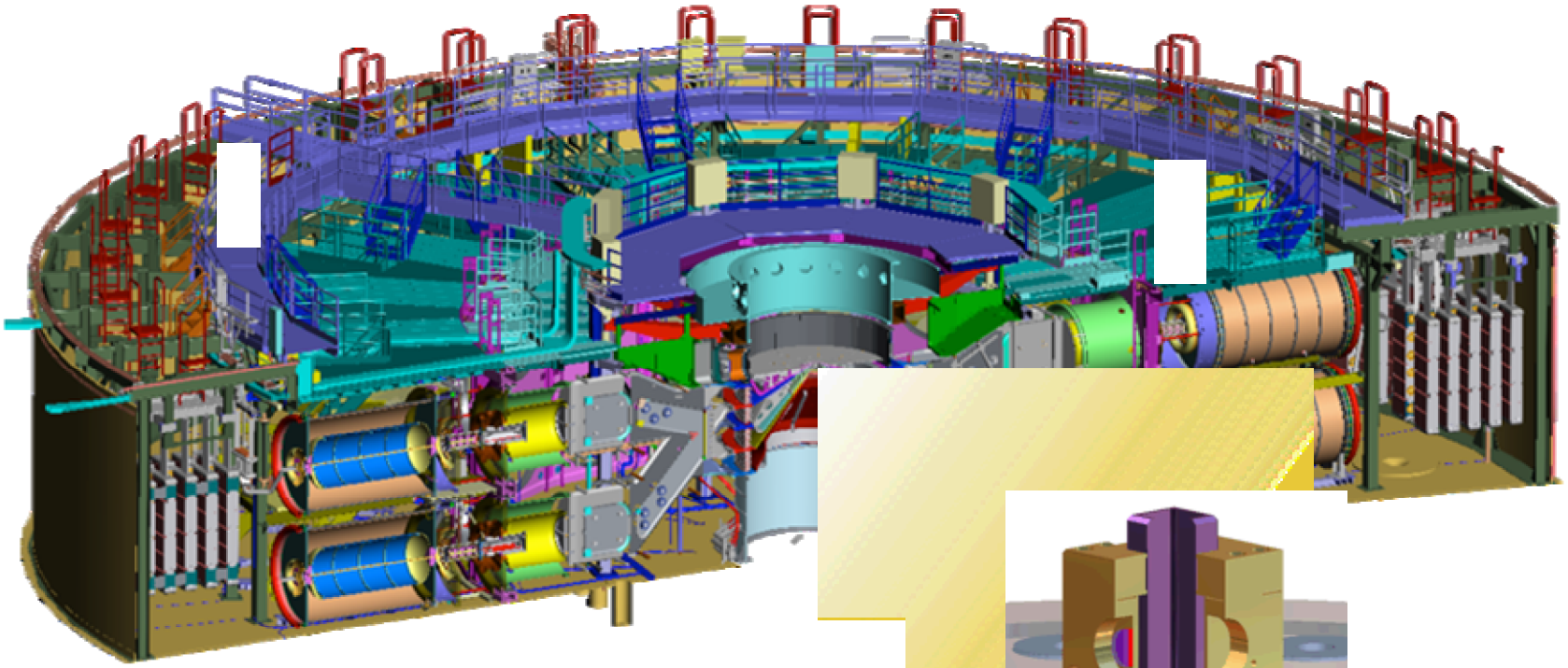


Laser-induced compression

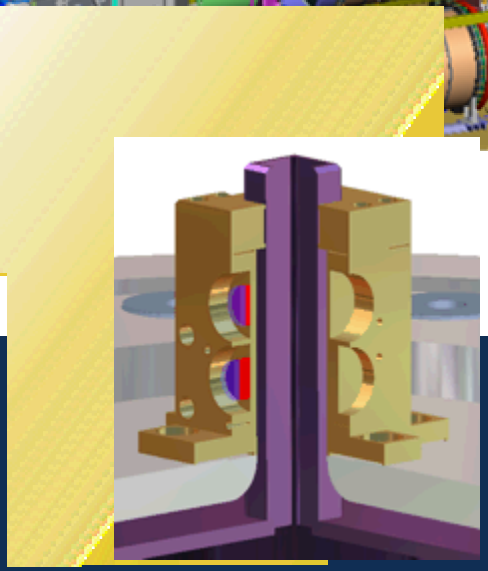
National Ignition Facility / LLNL

Courtesy of R. Hemley, Carnegie Institution of Washing

Sandia's Z accelerator is a unique platform for multi-mission research in high energy density (HED) environments



- Pulsed Power Technology
- Magnetically Driven Implosions
- Inertial Confinement Fusion
- Dynamic Compression of Materials



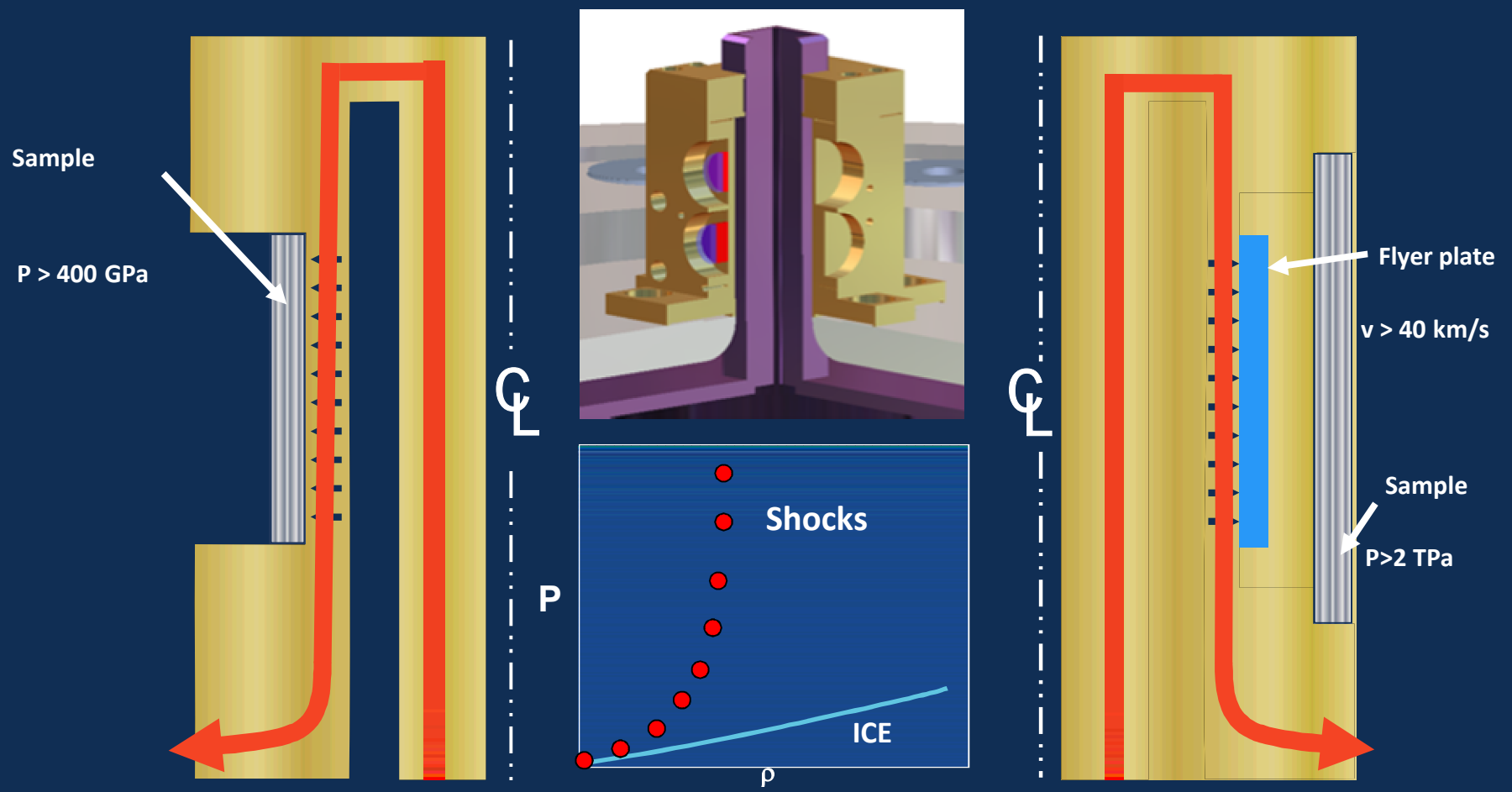
of state

I ~ 26 MA, τ ~100-1000 ns
X-ray power > 250 TW
X-ray energy > 2 MJ

Courtesy of D. Flicker, Sandia National Laboratories

Isentropic (ramp wave) compression and shock wave experiments explore different regions of phase space

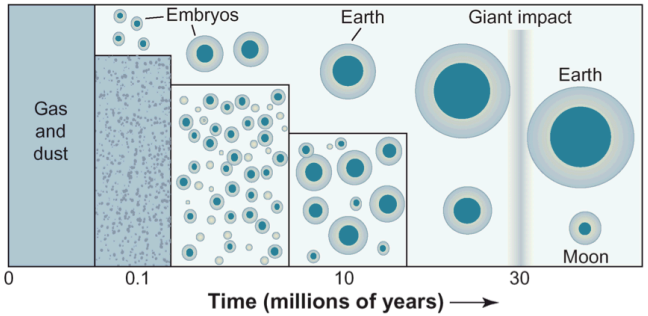
Courtesy of D. Flicker, Sandia National Laboratories



Isentropic Compression Experiments (ICE):
Gradual pressure rise in sample

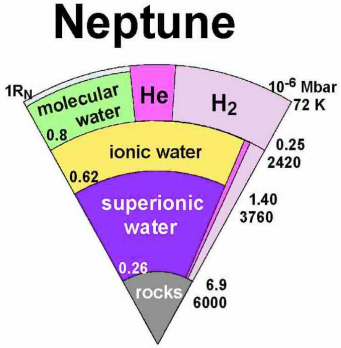
Shock Hugoniot Experiments:
Shock wave in sample on impact

The Z Fundamental Science Program forges strategic partnerships with leading institutions



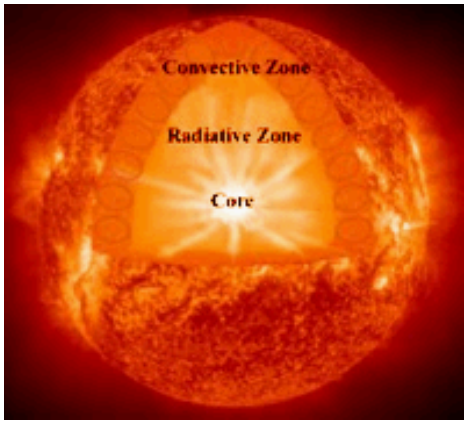
Earth and super earths

Properties of minerals and metals



Jovian Planets

Water and hydrogen



Stellar physics

Fe opacity and H spectra

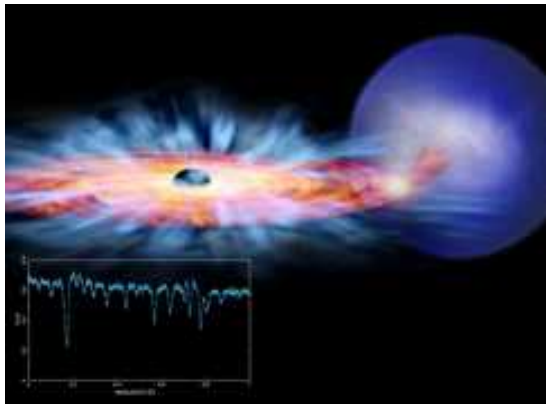


Photo-ionized plasmas

Range of ionization parameters

- Opportunities for collaboration and access to Z
- Competitive proposal process
- Science with significant impact
  - Bailey et al., Nature (2015)
  - Kraus et al., Nature Geoscience (2015)
  - Knudson et al., Science (2015)
- Annual workshops since 2009

Courtesy of D. Flicker, Sandia National Laboratories

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  - Materials for energy
  - Advanced manufacturing

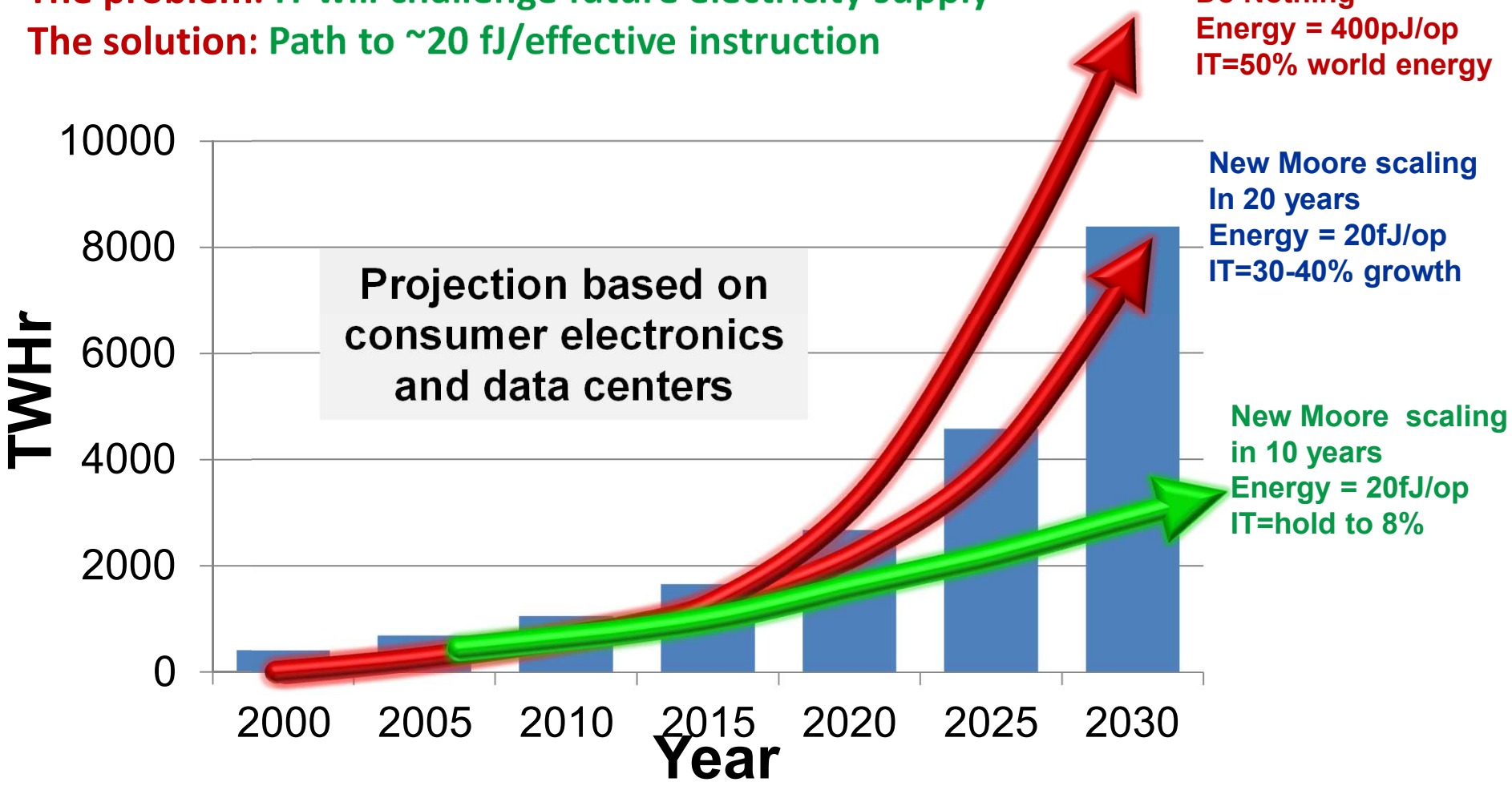
Student program at Sandia National Laboratories:

Beyond Moore's Law Computing – Seed funding available in FY2018
A DOE Big Idea to advance low-power computing

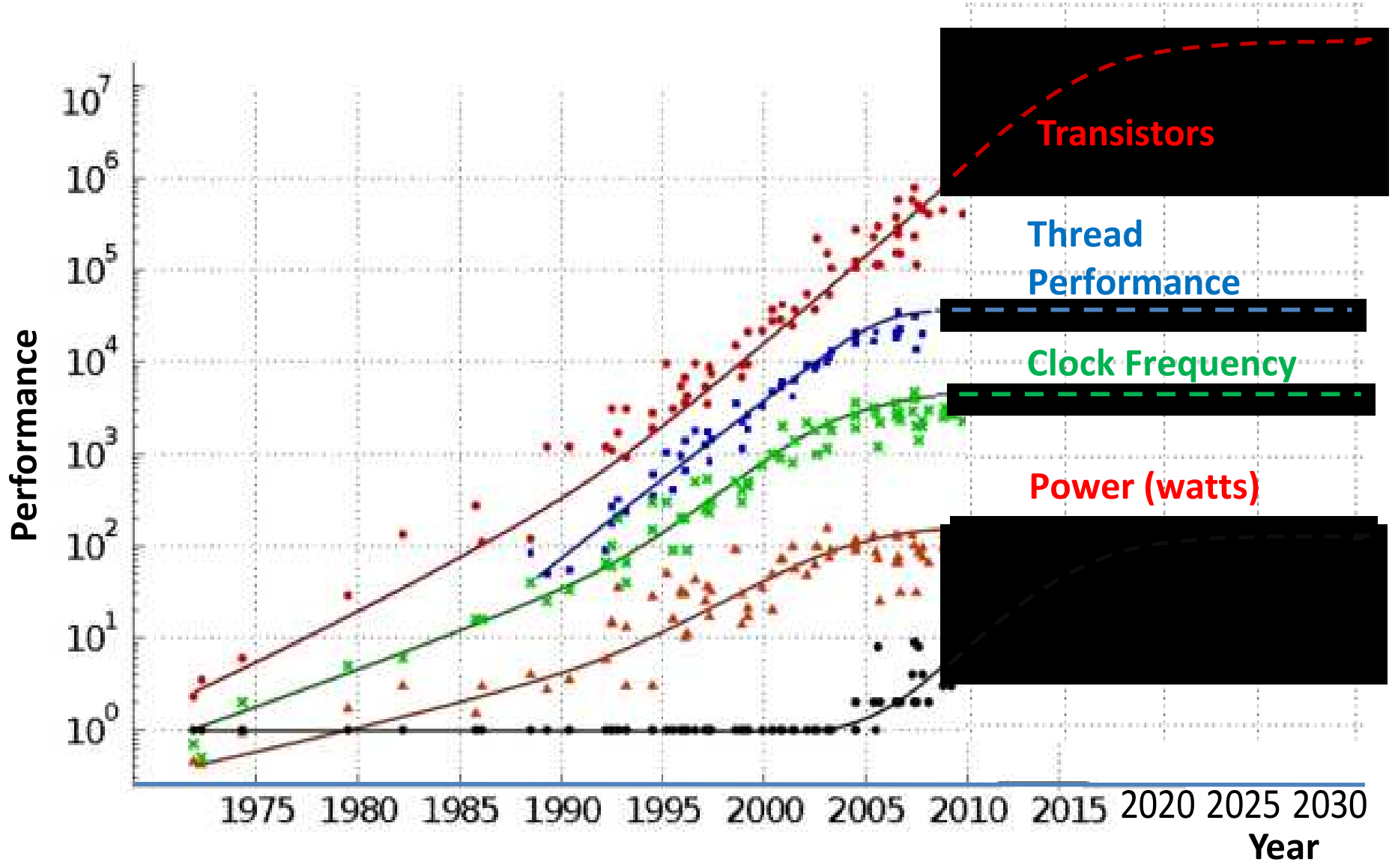
The opportunity: Administration's priority in high-performance computing (HPC)

The problem: IT will challenge future electricity supply

The solution: Path to ~20 fJ/effective instruction



Technology Scaling Trends:
Traditional sources of improvement have reached a plateau



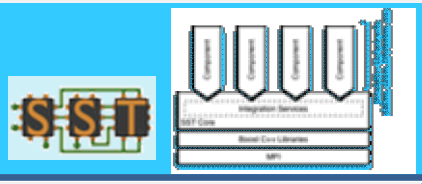
Multi-Scale Co-Design (MSDC) Framework

Modeling | **Experimental**

Algorithms & SW Environments

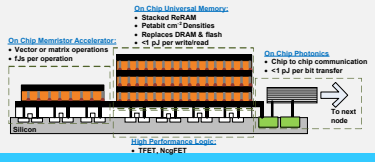
Algorithms and Software Environments
- **Application Performance Modeling**

Computer System Architecture Modeling
- Next generation of Structural Simulation Toolkit
- Heterogeneous systems HPC models



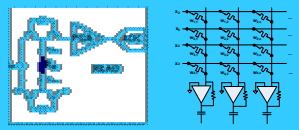
Hardware & Circuit Architectures

Microarchitecture Models
- McPAT, CACTI, NVSIM, gem5



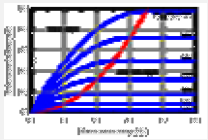
Component Fabrication
- Processors, ASICs
- Photonics
- Memory

Circuit/IP Block Design and Modeling
- SPICE/Xyce model



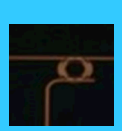
Comm., Memory & Computation Devices

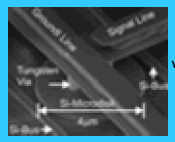
Compact Device Models
- Single device electrical models
- Variability and corner models

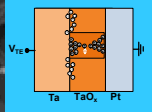


Device Measurements
- Single device electrical behavior
- Parametric variability

Device Physics Modeling
- Device physics modeling (TCAD)
- Electron transport, ion transport
- Magnetic properties



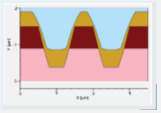


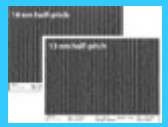


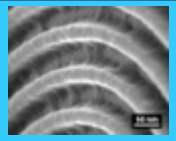
Device Structure Integration and Demonstration
- Novel device structure demonstration

Materials

Process Module Modeling
- Diffusion, etch, implant simulation
- EUV and novel lithography models

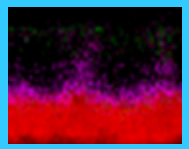






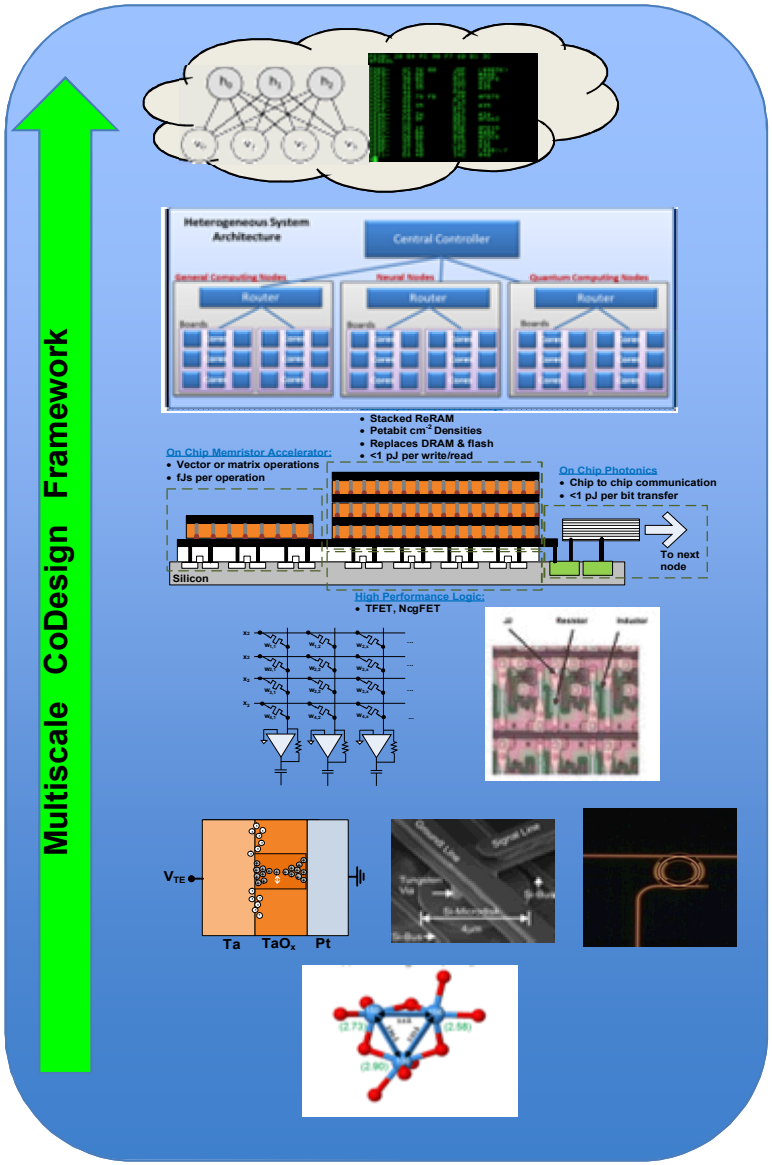
Process Module Demonstrations
- EUV and novel lithography
- Diffusion, etch, implant simulation

Atomistic and Ab-Initio Modeling
- **DFT – VASP, Socorro**
- MD – LAMMPS



Fundamental Materials Science
- **Understanding Properties/Defects via Electron, Photon, & Scanning Probes**
- **Novel Materials Synthesis**

The DOE NLs bring unique capabilities and competencies to implement the MSCD approach



CERI

NERSC

CSRI
Computer Science Research Institute

COMPUTER ARCHITECTURE LABORATORY
EXASCALE DESIGN SPACE EXPLORATION

SEQUOIA

ASC

AIM photonics

MOLECULAR FOUNDRY

CNI

CXRO
THE CENTER FOR X-RAY OPTICS

OAK RIDGE National Laboratory | CENTER FOR NANOPHASE MATERIALS SCIENCES

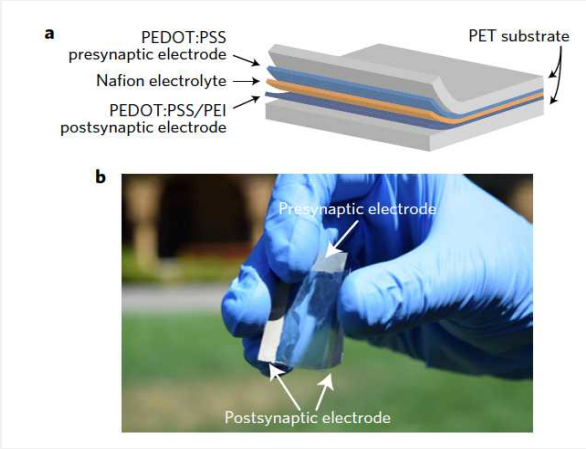
ALS

Argonne NATIONAL LABORATORY
Center for Nanoscale Materials

Sandia's competency in ionic transport leads to new microelectronic devices for low-power computing

Materials for non-conventional computing

- **Beyond Moore's Law Computing (BMC)**



Non-volatile organic synapse
Nature Materials (16), 2017

- **Opportunities:**
  - **Bio-inspired / neuromorphic computing**
  - **Quantum computing**

Sandia/CA is exploring neuromorphic transistors for ultra low-power computing (A. Talin/E. Fuller – 8342)

MRS Bulletin

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LETTERS
PUBLISHED ONLINE: 20 FEBRUARY 2017 | DOI: 10.1038/NMAT4856
nature materials

A non-volatile organic electrochemical device as a low-voltage artificial synapse for neuromorphic computing

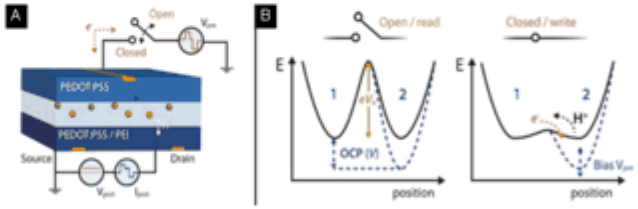
Yoeri van de Burgt[1†], Ewout Lubberman[1,2†], Elliot J. Fuller[3], Scott T. Keene[1], Grégorio C. Faria[1,4], Sapan Agarwal[3], Matthew J. Marinella[5], A. Alec Talin[3]* and Alberto Salleo[1]*

Biological, Biomedical, Biomaterials

Device mimics brain synapses

By F. Pelayo García de Arquer June 13, 2017

The human brain is arguably an intriguing and fascinating *computer*. Despite the slower speeds of neurons as compared to modern transistors, the brain still outperforms the best supercomputers in common tasks such as picture recognition. A challenge yet to be met is implementing systems that, inspired by the brain's working mechanism, are capable of efficiently solving complex problems.



Low-power artificial device based on organic flexible materials that can mimic brain synapses: (a) device architecture, consisting of two PEDOT layers separated by an ion transport membrane; and (b) schematic of the "read" and "write" operations, where protons are transferred from one electrode to the other depending on an applied voltage pulse. Credit: Nature Materials

Researchers from Stanford University and Sandia National Laboratories have realized a device capable of mimicking brain synapses that operates with remarkably low power consumption. Their system, which relies on inexpensive and flexible materials, turned out to be particularly efficient when implemented in neural network simulations. This work, carried out by the teams of Alberto Salleo at Stanford and Alec Talin at Sandia Labs, was published in *Nature Materials*.

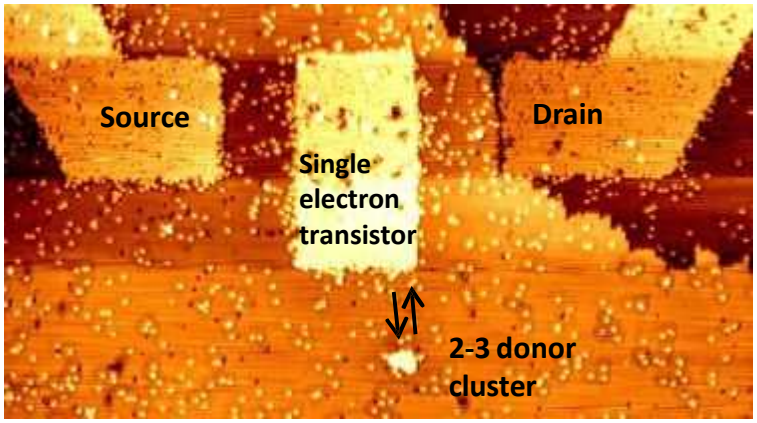
Outline

- Overview of Sandia National Laboratories:
  - Mission
  - Scientific capabilities and core competencies
  - Research infrastructure

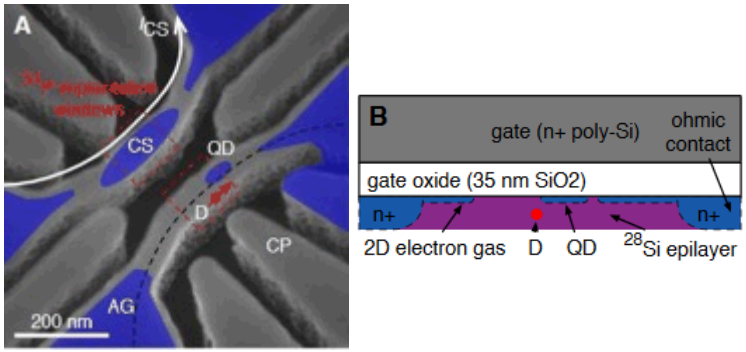
- **Materials science opportunities at Sandia:**
  - Materials in extreme environments
  - Materials for non-conventional computing
  - **Quantum materials**
  - Materials for energy
  - Advanced manufacturing

Student program at Sandia National Laboratories:

Atomic-Precision Lithography for Quantum Information Science



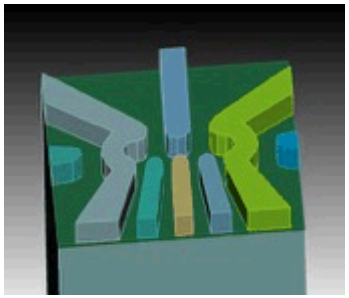
Atomic-precision silicon donor devices

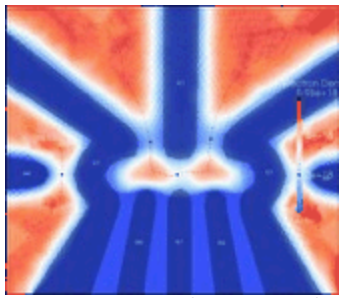


Coupled donor-quantum dot devices

- Sandia 2nd lab worldwide, 1st in US to demonstrate atomic-precision Si lithography

M. Rudolph, APL 105, 163110 (2014)
P. Harvey-Collard, arXiv:1512.01606
X. Gao, JAP 114, 164302 (2013)



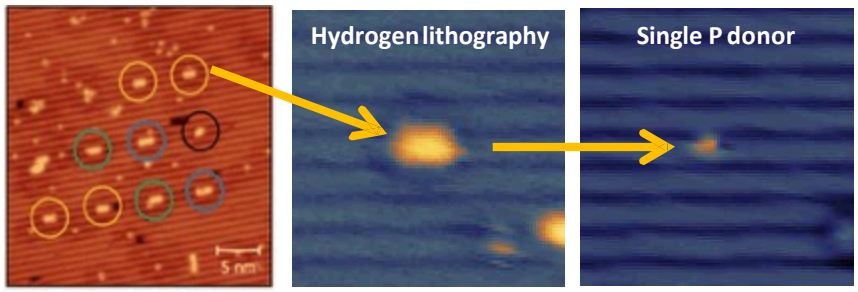


Electron Density (red = higher)

Quantum Computer Aided Design - QCAD

Courtesy of J. Nelson, Sandia National Laboratories

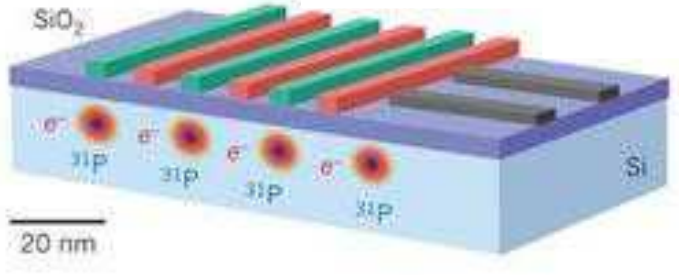
Atomic-Precision Lithography for Strongly Correlated Electron Systems



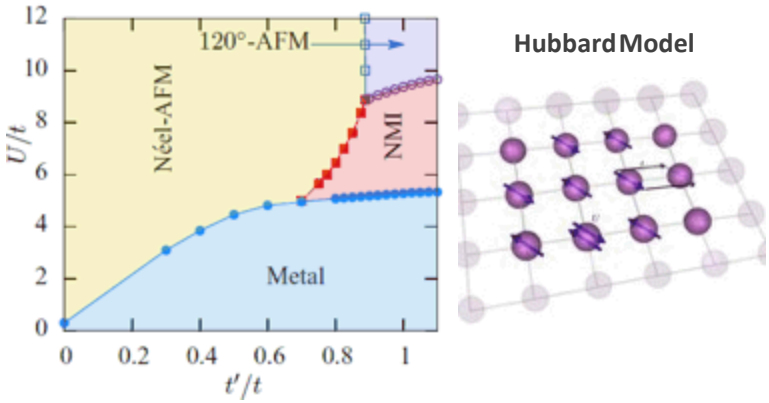
Single-donor placement with atomic precision

- **Ability to create atomic-precision electronics opens doors to new fundamental science**

Shashank Misra, Dan Ward, Dwight Luhman, Lisa Tracy, Tzu-Ming Lu, Jonathan Moussa, Andrew Baczewski



Hubbard lattice of donors = Artificial strongly correlated materials



M. Laubach et al, Phys. Rev. B 91, 245125 (2015)

Courtesy of J. Nelson, Sandia National Laboratories

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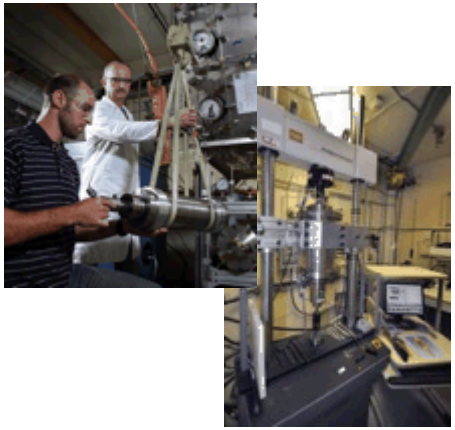
  - Quantum materials
  - **Materials for energy**
  - Advanced manufacturing

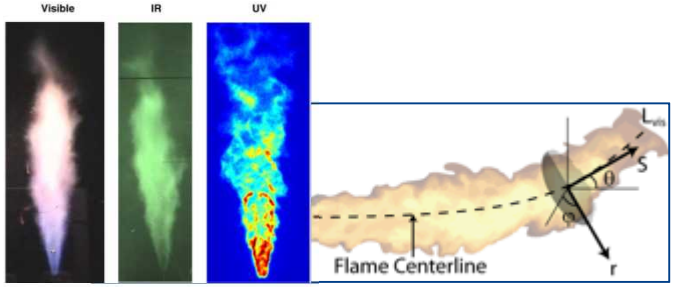
Student program at Sandia National Laboratories:

Hydrogen science and engineering for transportation, nuclear security, and fusion energy – Sandia/CA

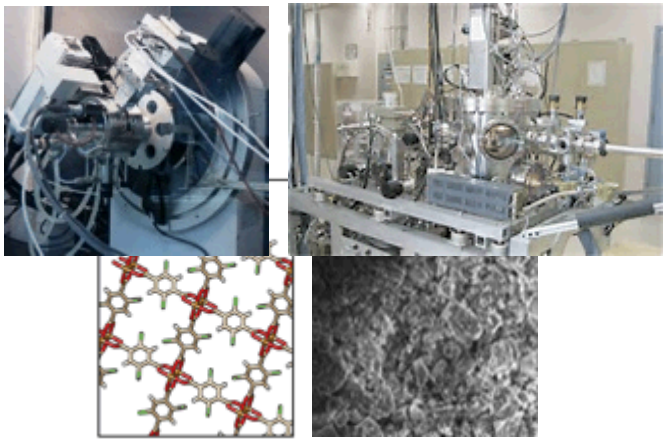


Material fracture and fatigue in high-pressure environments

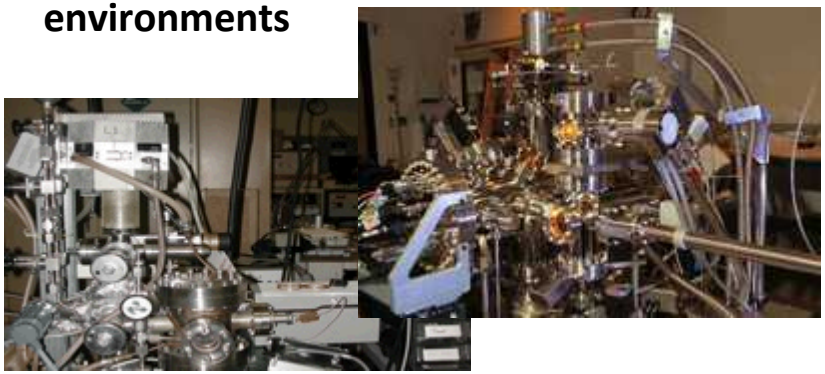
HyRAM
HYDROGEN RISK ASSESSMENT MODELS



Risk-informed safety standards, built on rigorous scientific observations and models



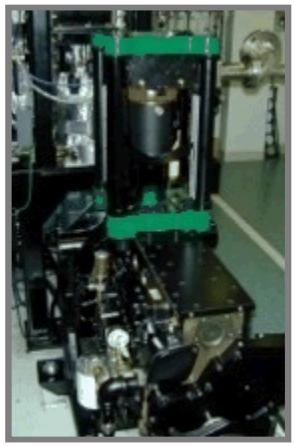
Materials discovery



Hydrogen adsorption and permeation

Engineered systems and innovative applications

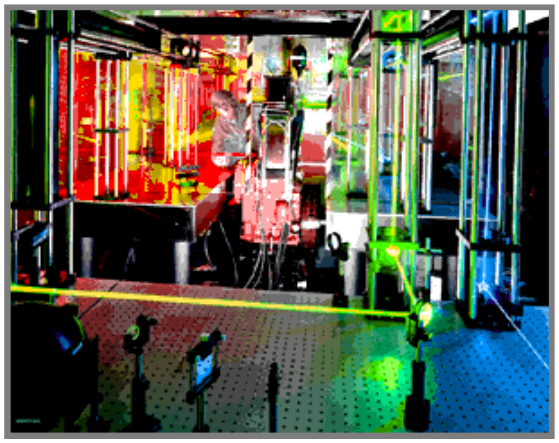
Engine combustion research at Sandia/CA



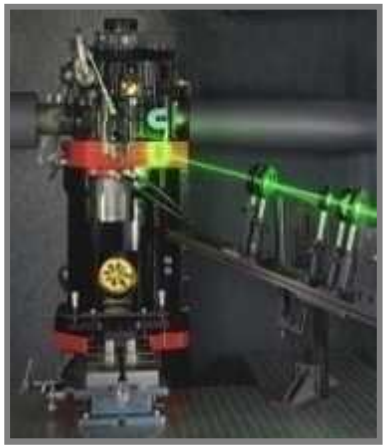
Low-temperature gasoline combustion

Alternative fuels – light-duty direct injection spark ignition

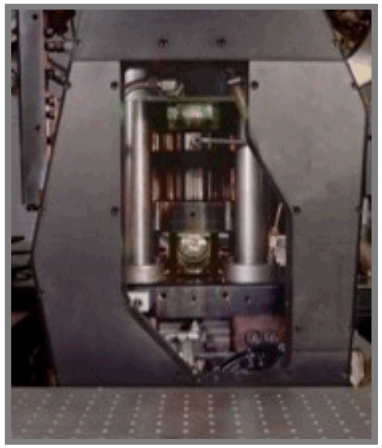
Spark ignition & combustion fundamentals



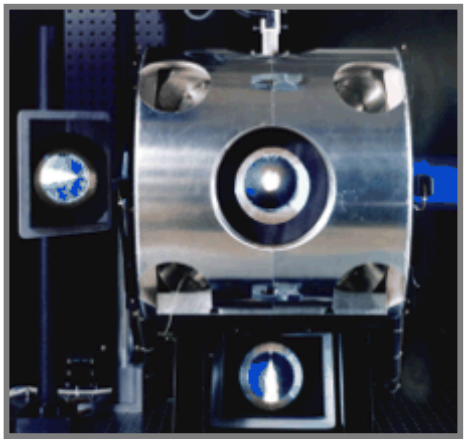
Alternative fuels – heavy-duty compression ignition



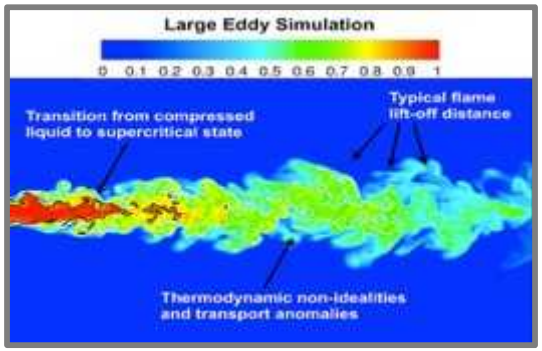
Heavy duty Diesel LTC diesel combustion



Light duty Diesel LTC diesel combustion



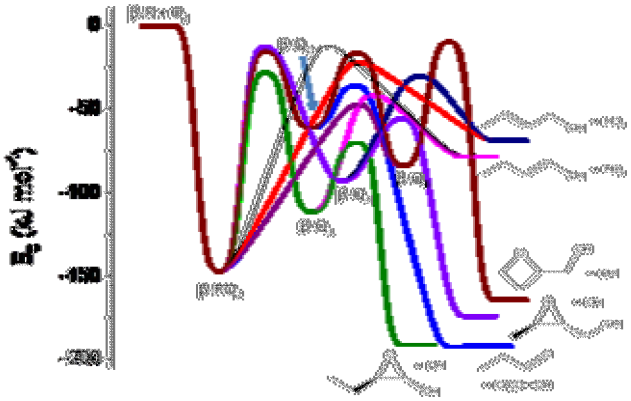
Fuel sprays

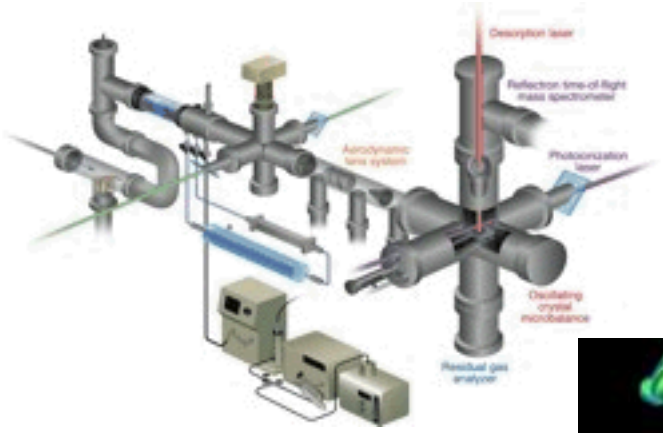


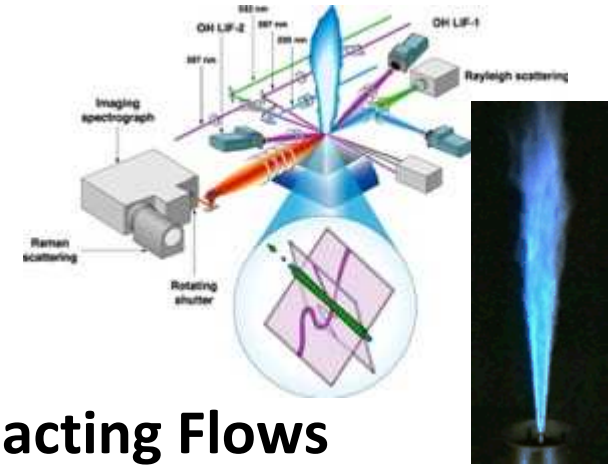
Computational simulation of engine processes

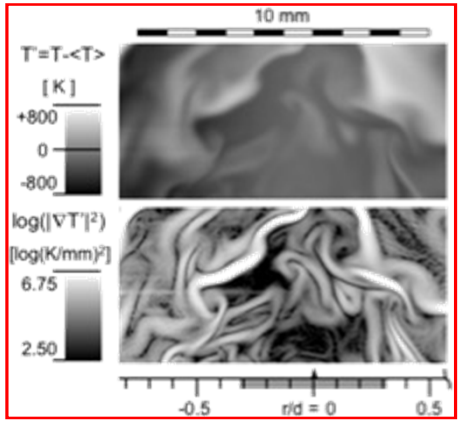
Chemical sciences research at Sandia/CA

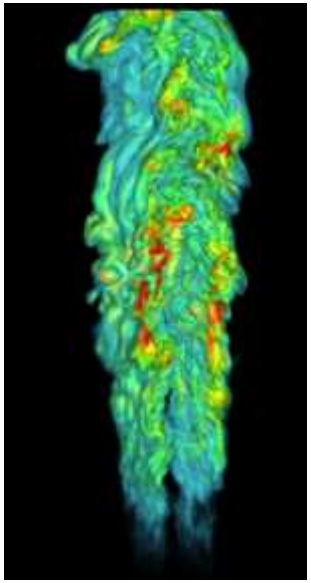
Combustion Chemistry and Diagnostics











Reacting Flows

Outline

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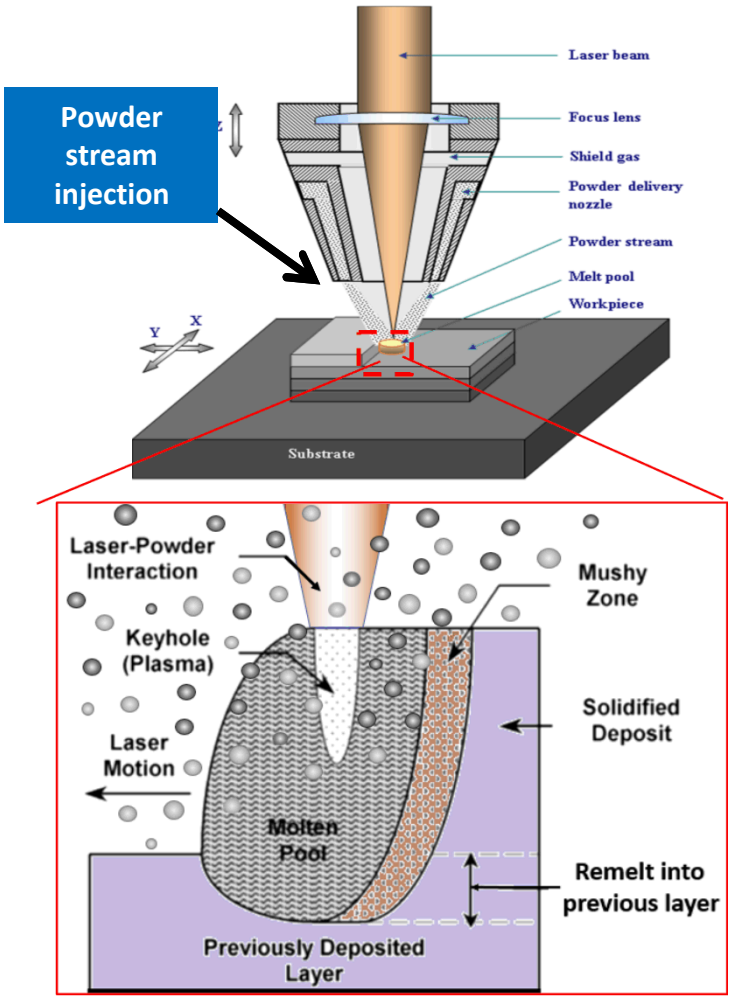
  - Materials for energy
  - **Advanced manufacturing**

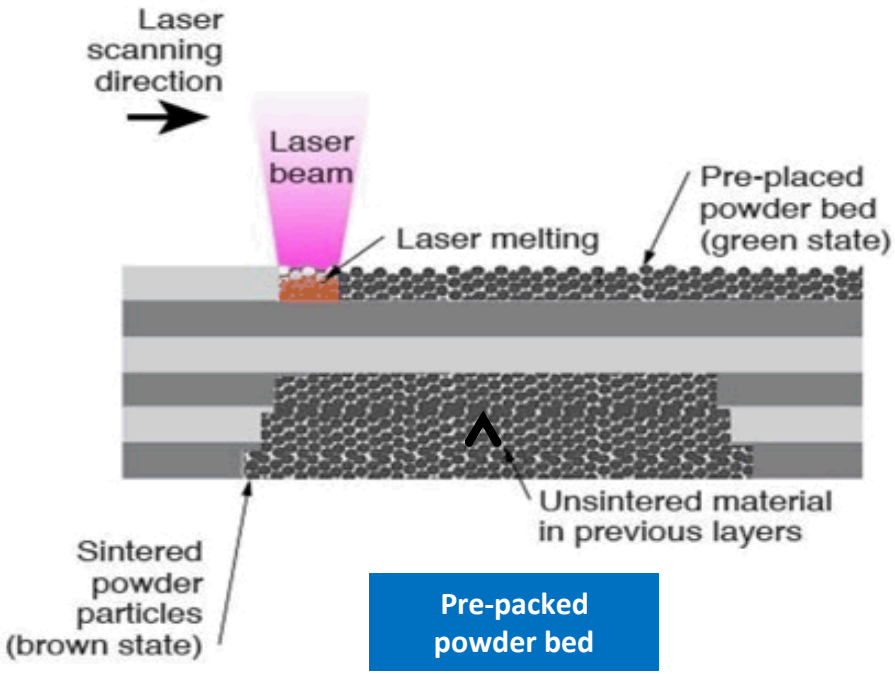
Student program at Sandia National Laboratories:

Additive Manufacturing (AM) printing:
Synthesizing 3D objects by fusing/binding/melting successive layers of materials

Laser Engineered Net Shaping (LENS)



Powder Bed Fusion (PBF)

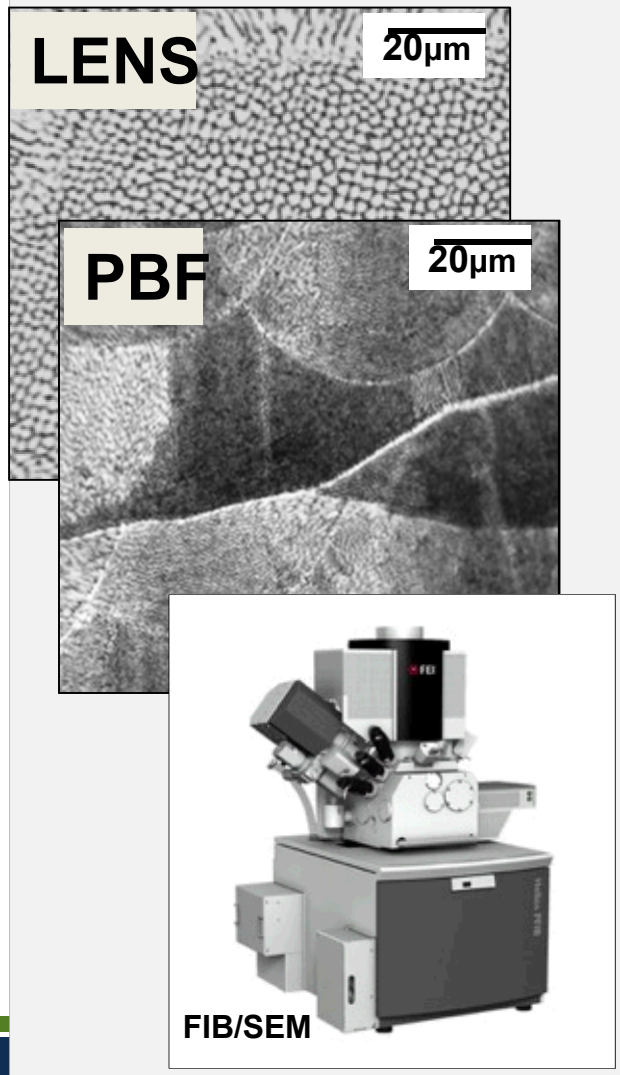


Processes for LENS & PBF

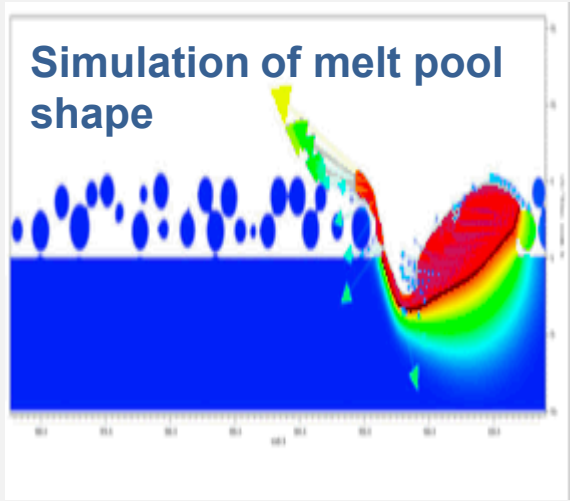
- Powder melting
- Molten metal fusion
- Molten metal solidification

Additive manufacturing (AM) presents unique opportunities to advance processing science, modeling/simulation, and testing/characterization

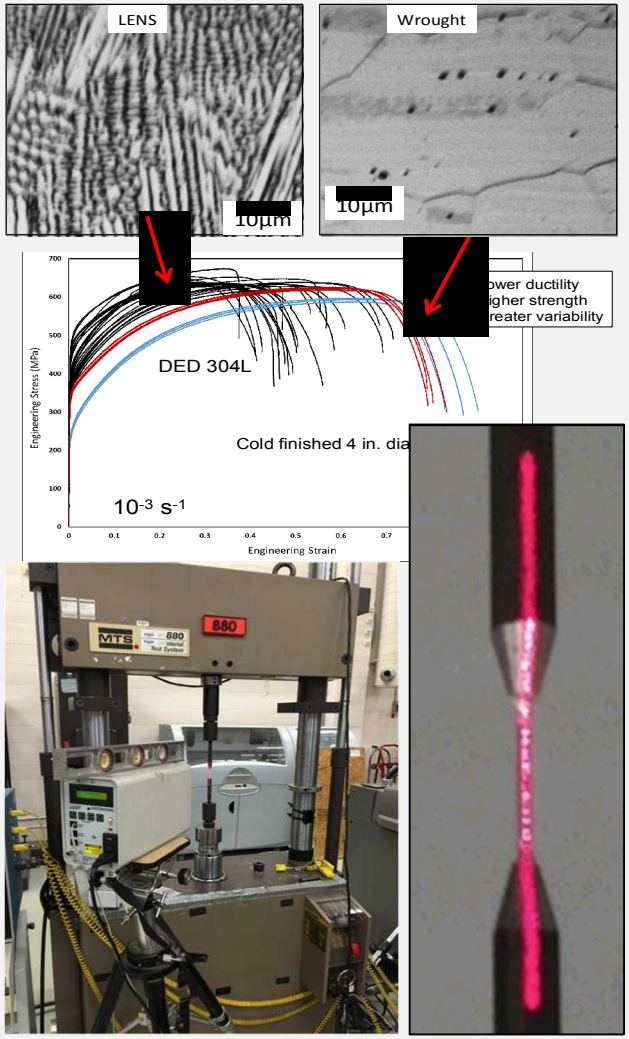
Synthesis and Characterization



Modeling and Simulation

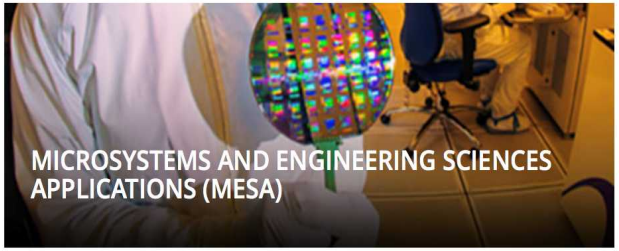


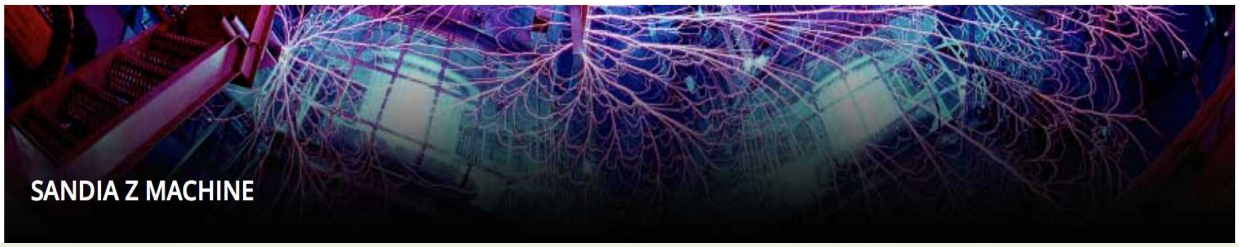
Mechanical Testing



Visit Sandia National Laboratories in CA and NM:

http://tours.sandia.gov/tours.html





Students/postdocs program at Sandia National Laboratories:

http://www.sandia.gov/careers/students_postdocs/

BACKUPS