SAND2014-15381PE

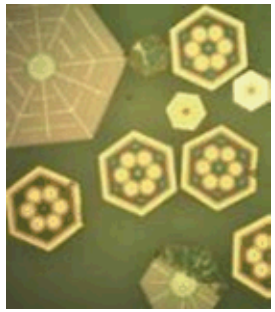
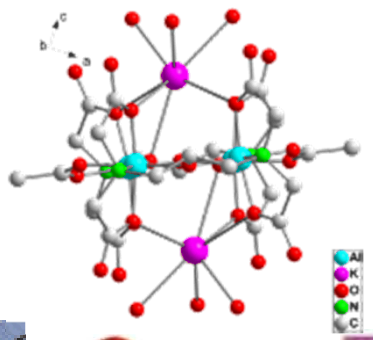
Exceptional service in the national interest

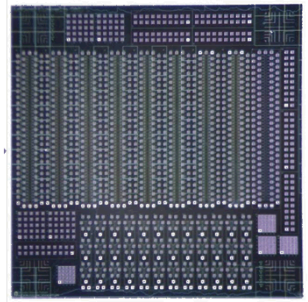
Sandia National Laboratories

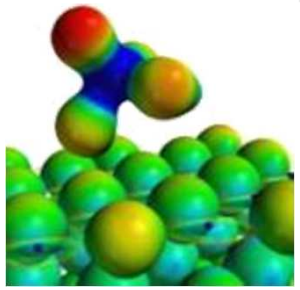
Energy Research Program Area - Energy & Climate Program

J. Charles Barbour,
Program Area Director
jcbarbo@sandia.gov

25 June 2014



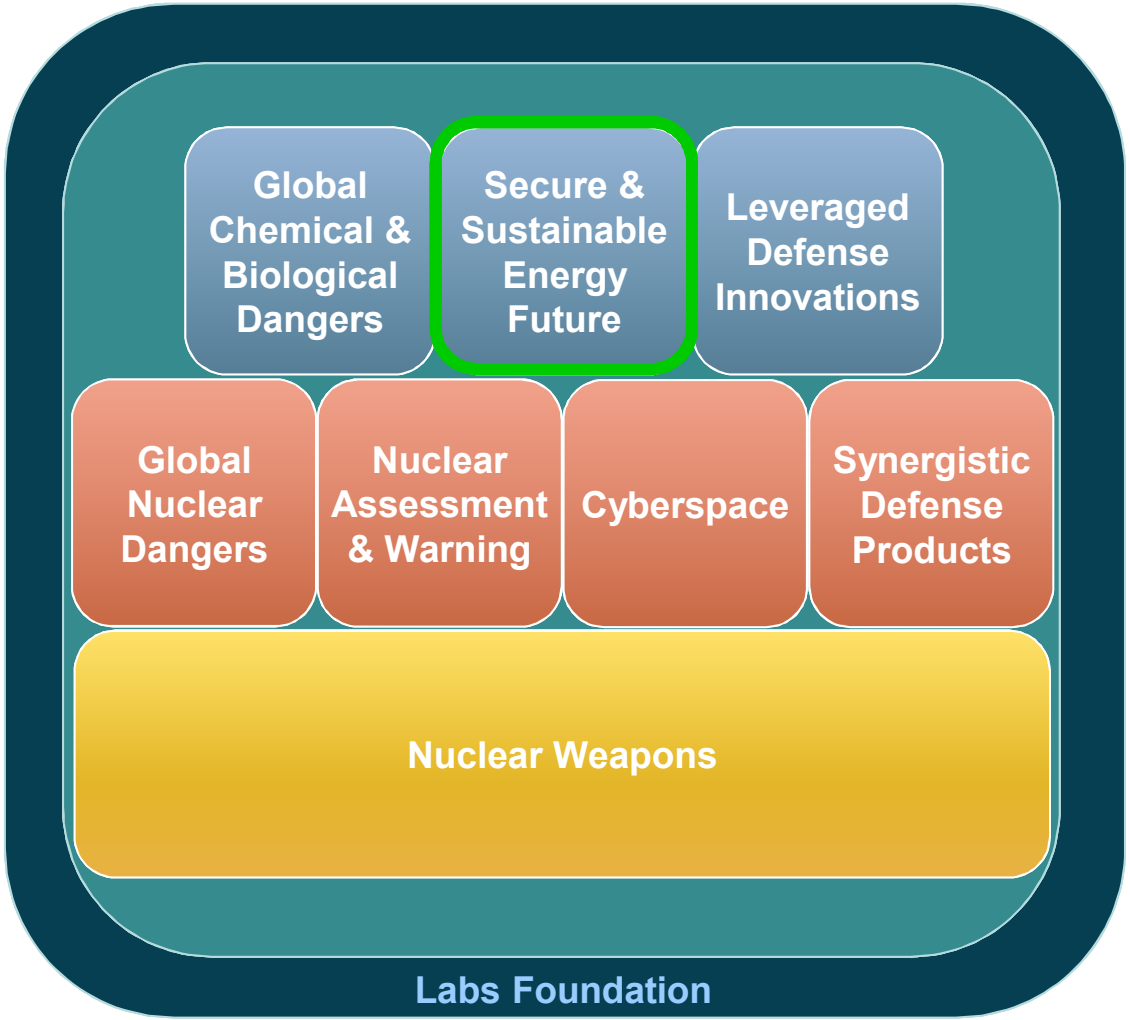



U.S. DEPARTMENT OF ENERGY

NNSA

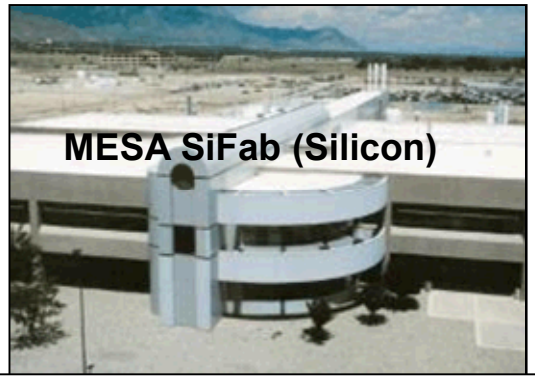
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia Mission Areas Set the Strategy



Differentiating facilities at Sandia

Sandia National Laboratories



MESA = Microsystems Engineering, Science, and Applications

Unique combination of state-of-the-art laboratories/facilities: materials growth, device & nanosystem / microsystem fabrication, *in-situ* characterization (structural, electronic, and optical), HPC.

Energy & Climate Program Areas

Sandia National Laboratories

Renewable Systems & Energy Infrastructure

PAD: Carol Adkins
Deputy: Juan Torres

- **Renewable Energy** — Juan Torres
- **Energy Efficiency** — Imane Khalil
- **Grid & Storage Systems** — Sean Hearne

Nuclear Energy & Fuel Cycle Program

PAD: Peter Davies
Deputy: Erik Webb

- **Commercial Nuclear Power & Fuel** — Tito Bonano
- **Nuclear Energy Safety & Security** — Susan Pickering
- **DOE Managed Nuclear Waste Disposal** — Paul Shoemaker

Transportation Energy & Systems

PAD: Bob Hwang
Deputy: Art Pontau

- **Vehicle Technologies** — Art Pontau
- **Biomass Technology** — Blake Simmons
- **Fuel Cells/Hydrogen Technology** — Daniel Dedrick

Climate & Environment

PAD: Marianne Walck
Deputy: Amy Halloran

- **Measurements & Modeling** — Scott Collis
- **Carbon Management** — Erik Webb
- **Water & Environment** — Stephanie Kuzio
- **Biofuels** — Blake Simmons

Energy Research

PAD: Charles Barbour
Deputy: Jerry Simmons

- **ARPA-e** — Wahid Hermina
- **SC BES CHEMSCIENCE** — Dawn Manley
- **SC ASCR** — Scott Collis
- **SC BES CINT** — Neal Shinn
- **SC BES GEO, BIOSCIENCE** — Erik Webb
- **SC BES MATERIALS SCIENCES** — Richard Schneider

Energy Research Vision

Sandia National Laboratories

Be the leaders that change the scientific community in:

- ***Predictive Models for Combustion***
- ***Integrated Nanosystems - Quantum electronics to nanomaterials behavior***
- ***Predictive performance of subsurface carbon capture***
- ***Computational science of uncertainty quantification & math algorithms***
- ***HPC architectures for exascale computing***

Use strength in scientific competencies to differentiate our mission work

Office of Science Research

One of the few program areas at Sandia that supports the scientific base for competencies essential to Sandia missions.

Office of Science
U.S. Department of Energy

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

arpa·e
CHANGING WHAT'S POSSIBLE

Enabling Research Program Area Goals

Sandia National Laboratories

- Nurture discovery science for fundamental breakthroughs and deepen our competencies in key strategic areas that enable ECIS mission objectives and goals.
- Accelerate industry development of transformational energy technologies through ARPA-E
- Pioneer advanced electrical energy storage technologies and develop new technologies for enhanced battery safety and reliability, through scientific research in materials and chemistry, and innovative architectures and cell designs.
- Enable analysis capabilities to inform and influence the nation's debate on energy strategy and policy.

Enabling Research Financial Summary

Sub-sub program area	FY14 Cost ($M)
ASCR	14.0
BES – Chemical Science	13.1
BES – CINT	11.9
BES - Materials Science	16.9
BES – Geoscience	1.8
FES + ICO	3.2
ARPA-E	0.8
Total	61.7

LDRD
ECIS LDRD costs $9.57M

Patents & Royalties **$1.6M**

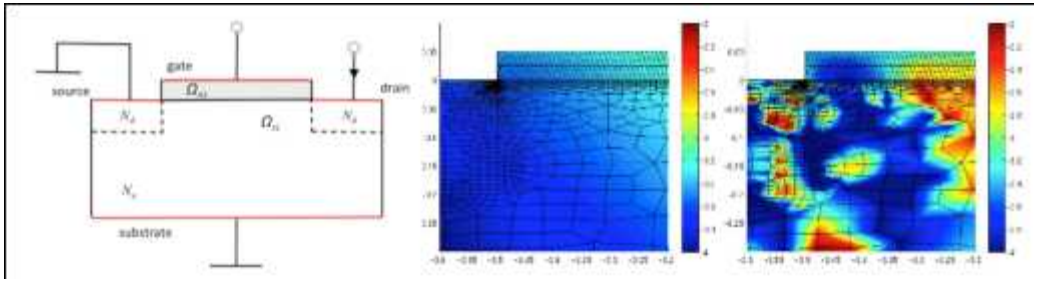
Advanced Scientific Computing Research (ASCR)

Sandia National Laboratories

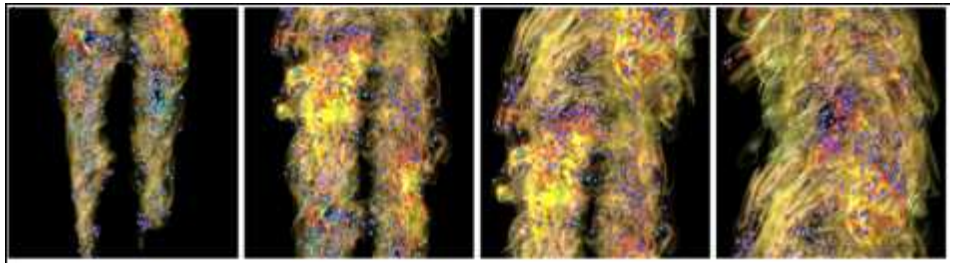
DOE/ASCR Applied Mathematics and Computer Science Research with Application to National-Scale Science

SciDAC Scientific Discovery through Advanced Computing

- **Applied Mathematics Research**
  - Uncertainty quantification
  - Multiscale mathematics
  - Scalable algorithms
  - Optimization of complex systems
- **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



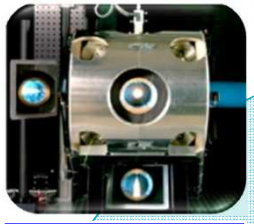
Rigorous mathematics leads to physical solutions for MOSFET device models (middle) compared to traditional methods that are unstable (right).



Volume and particle visualization from Combustion of methanol

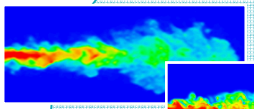
Basic Science Foundation for Predictive Combustion Models – BES / Chem. Science

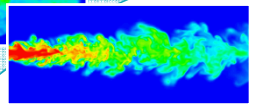
High Pressure Spray

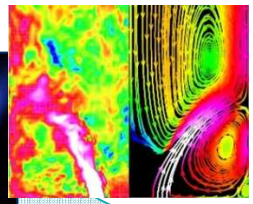


Device Validation

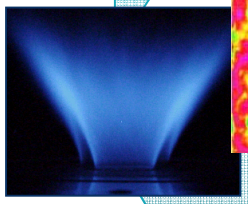
Predictive Engineering Models



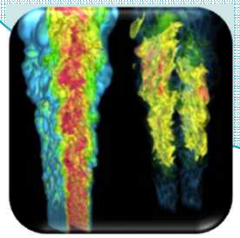




Large Eddy Simulation (LES)

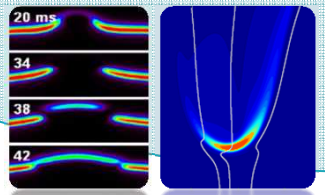


Turbulent Flame Experiments

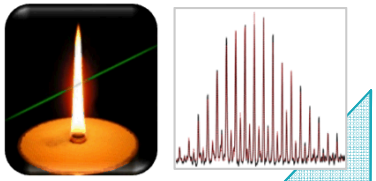


Direct Numerical Simulation (DNS)

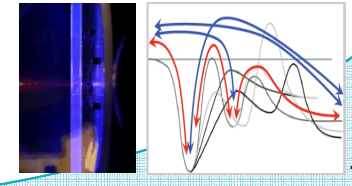
Laminar Experiments and Simulations



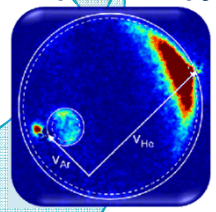
Optical Diagnostics



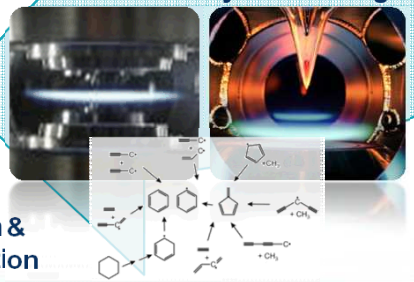
Elementary Chemical Kinetics



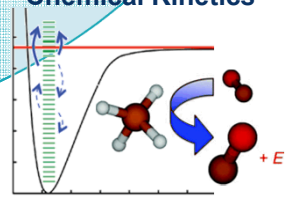
Chemical Dynamics & Spectroscopy



Flame Chemistry & Modeling

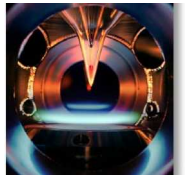


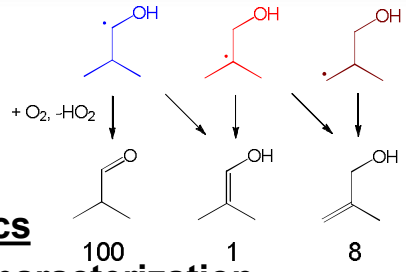
Theoretical Chemical Kinetics



Mechanism Reduction & Uncertainty Quantification

Science Vision





Unique Equipment

- Low pressure flames
- Turbulent reacting flows
- Molecular beam mass spectrometer
- High pressure laser photolysis
- High pressure soot reactor
- Jet-stirred reactor
- Multiphase jet & counterflow flames

Optical diagnostics

- Femtosecond
- High rep-rate imaging
- Laser-induced incandescence
- Tomographic particle image velocimetry

Uncertainty quantification

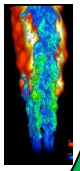
Platforms for idealized combustion environments

Basic science elements

Technique Development

Modeling

- Chemistry
- Quantum chemistry
- Transition state theory
- Mechanism development
- Turbulence-chemistry
- DNS and LES
- Soot
- Incipient formation
- Growth
- Multiphase

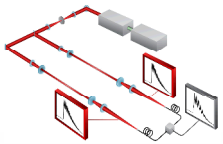


Chemical kinetics

- Radical characterization
- Non-adiabatic chemistry
- Chemical dynamics
  - Three body interactions
  - Collisional energy transfer
- Reacting flow theory
- Chemical mechanisms for soot oxidation & growth
- Chemistry and mixing in dense sprays and multiphase flows

Spectroscopy

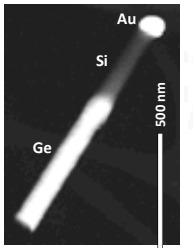
- VUV photoionization
- Coherent spectroscopies
- Dual etalon frequency comb
- Surface diagnostics
- Ambient press x-ray photoelectron
- Near-edge x-ray absorption fine structure



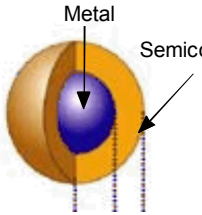
Center for Integrated Nanotechnologies (CINT)

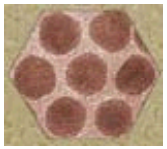
One scientific community focused on nanoscience integration

Nanoscale building blocks



Vapor & liquid phase synthesis



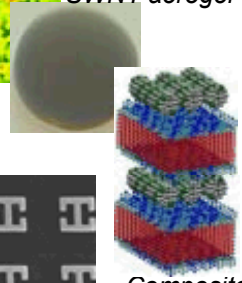


Heterostructuring & interface modification

Fabrication & assembly

Nanocomposite

SWNT aerogel

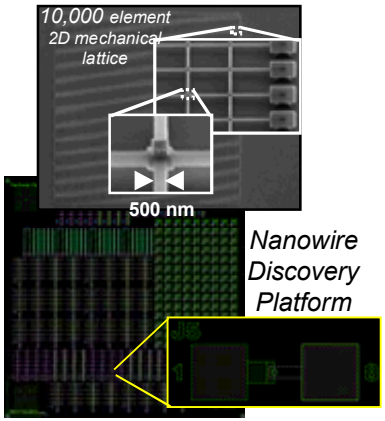


Composite membranes

Switchable metamaterials

Functional composites & systems

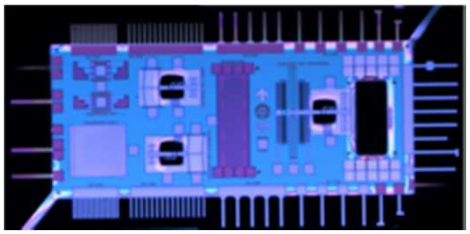
Nanomechanical arrays



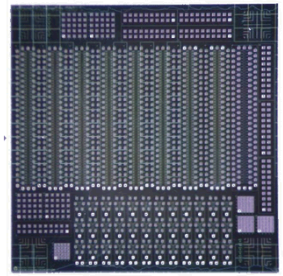
Length scale

Nano → Micro

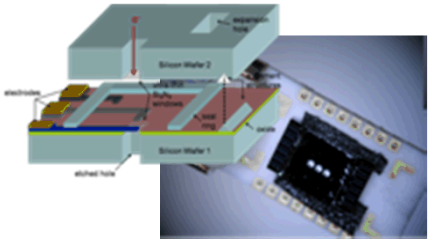
Understand and exploit differentiating properties at the nanoscale.



Nanomechanics & Thermal Transport

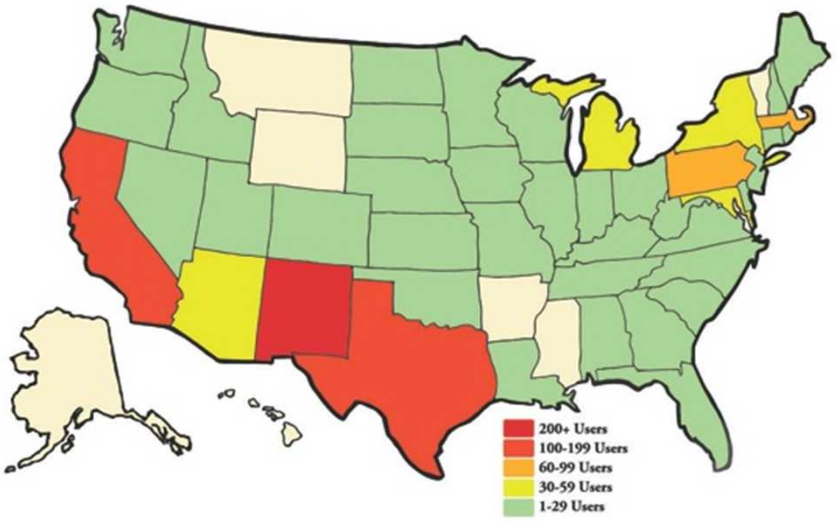


Nanowires



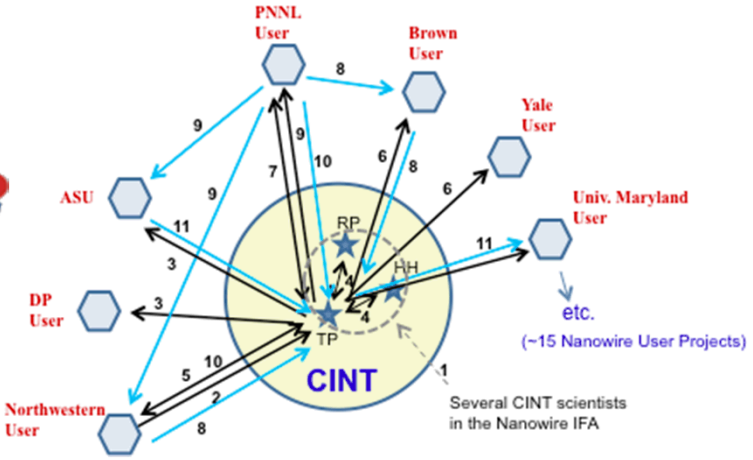
TEM Liquid Electrochemistry

CINT attracts a diverse community of users



User Institutions:

- Academic - USA (45%)
- Academic - Foreign (5%)
- LANL+SNL (30%)
- Other Gov't. Labs (15%)
- Industrial (5%)

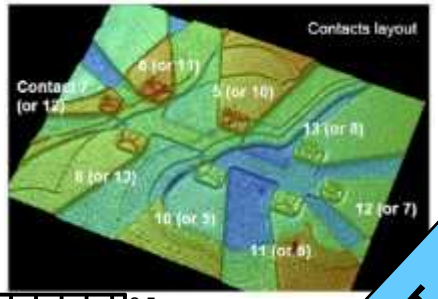


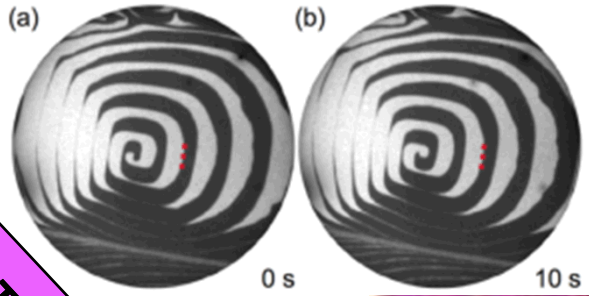
NanoBlox
Building Blocks for Nanotechnology
www.NanoBloxInc.com

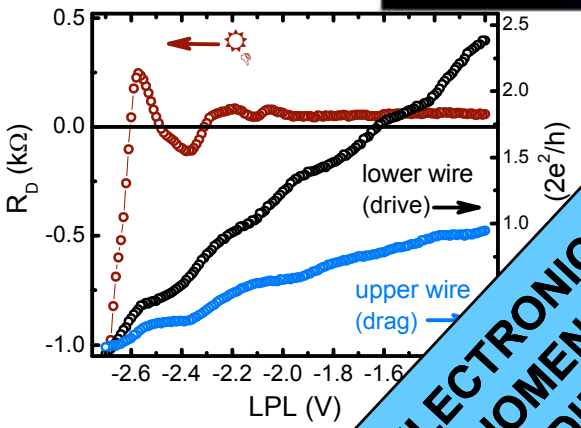
BES – Materials Science

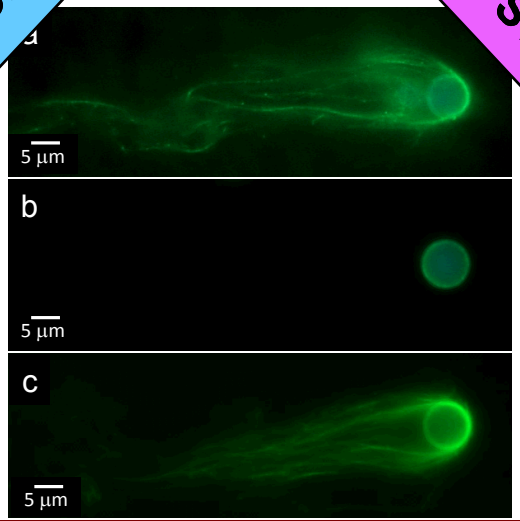
Discoveries Emerge at Nexus of Strengths

Sandia National Laboratories









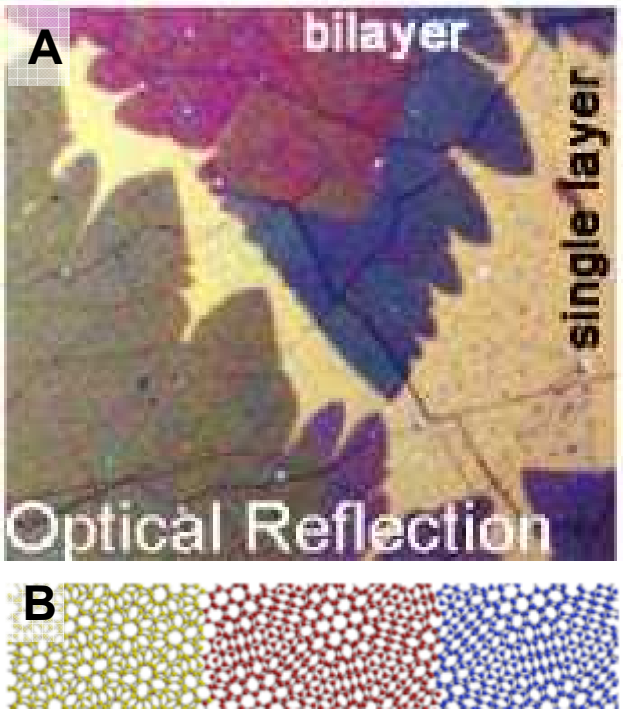
QUANTUM ELECTRONICS, EMERGENT COLLECTIVE PHENOMENA, SEMICONDUCTOR MATERIALS, LOW-DIMENSIONAL PHYSICS

INTERFACE SCIENCE, MOLECULAR COMPOSITES, ATOMIC SCALE SELF-ASSEMBLY, INTERFACIAL MECHANICS, STRUCTURE AND DYNAMICS

13

Optical Properties of Twisted Bilayer Graphene

Sandia National Laboratories



A) Optical image of the "stained-glass window" appearance of twisted bilayer graphene on oxide-covered silicon, (B) Schematic illustration of the colored regions' atomic arrangement

Scientific Achievement

Bilayer graphene films exhibit a "stained-glass window" appearance explained by the emergence of a narrow absorption band in the visible spectrum that depends on the azimuthal misorientation between layers.

Significance and Impact

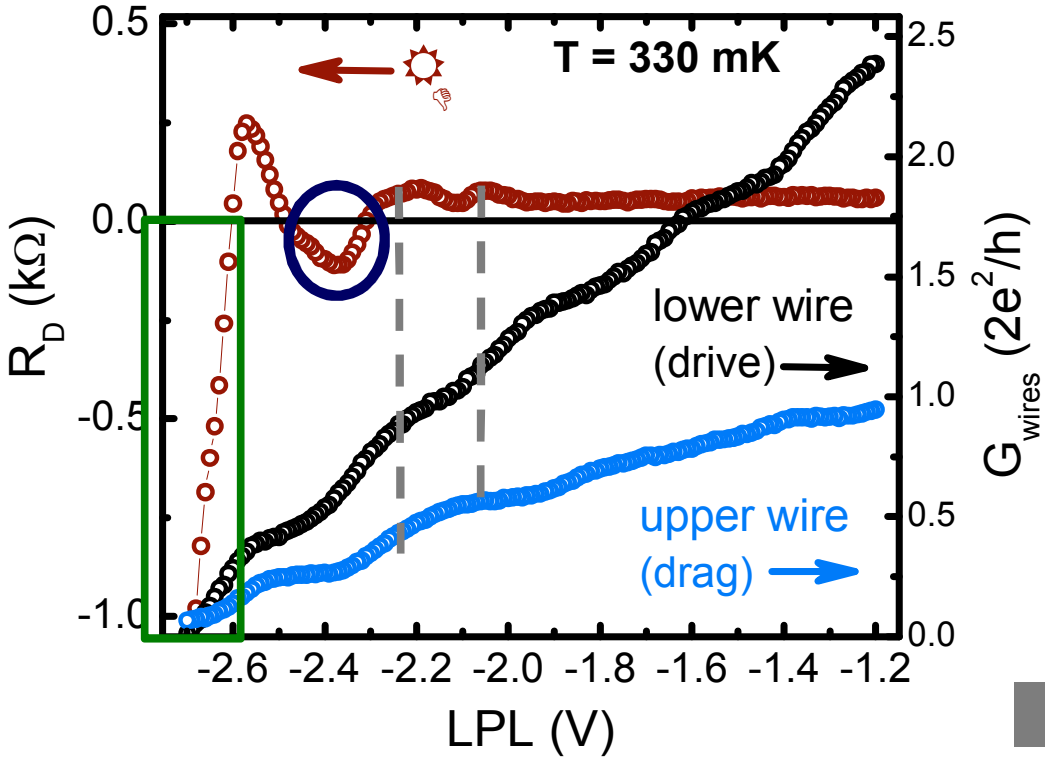
The ability to tune the optical properties of ultrathin layers has promising implications for sensing devices and optical filters.

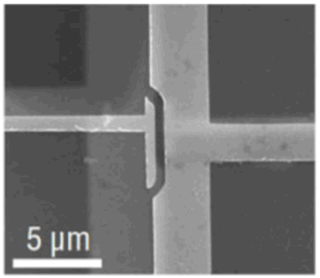
Research Details

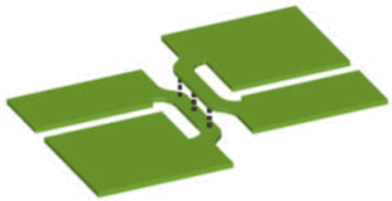
- The structures were fabricated by two direct transfers of graphene sheets onto a silicon dioxide substrate
- The transfer produced clean interfaces over large areas
- Stacking the sheets with a twist angle leads to direct electronic interactions between layers
- These interactions give rise to color variations

J.T. Robinson[1], S.W. Schmucker[1], C. B. Diaconescu[2], J. P. Long[1], J.C. Culbertson[1], T. Ohta[2], A. L. Friedman[1], T. Beechem[2], Electronic Hybridization of Large-Area Stacked Graphene Films, ACS Nano 7, 637 (2013) & Science 152, 374 (2013) [1] = NRL, [2] = SNL

Coulomb Drag Between Vertically-Integrated Quantum Wires







Scientific Achievement

A totally unexpected re-entrant negative Coulomb drag was observed in coupled quantum wires.

Significance and Impact

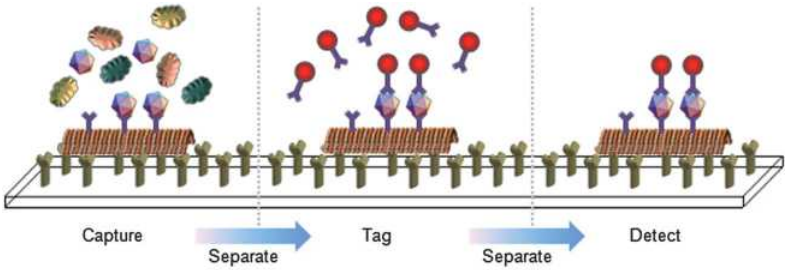
Results are expected to lead to deeper understanding of Luttinger physics in 1D systems where electron interactions and correlations are strong.

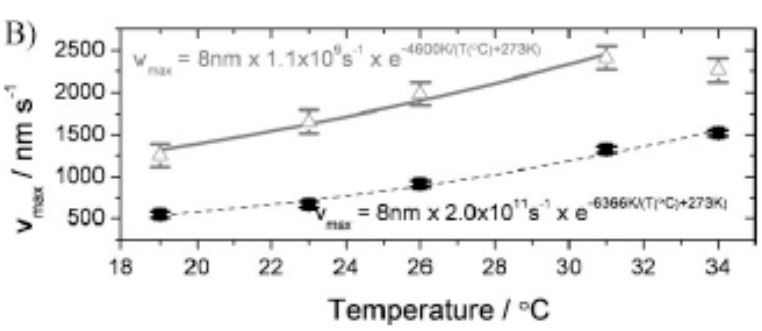
Research Details

- Peaks in the drag signal as 1D subbands get depleted
- Low-density negative drag observed when $N_{wires} < 1$
- Re-entrant negative drag when $N \geq 1$ in both wires, never observed previously.

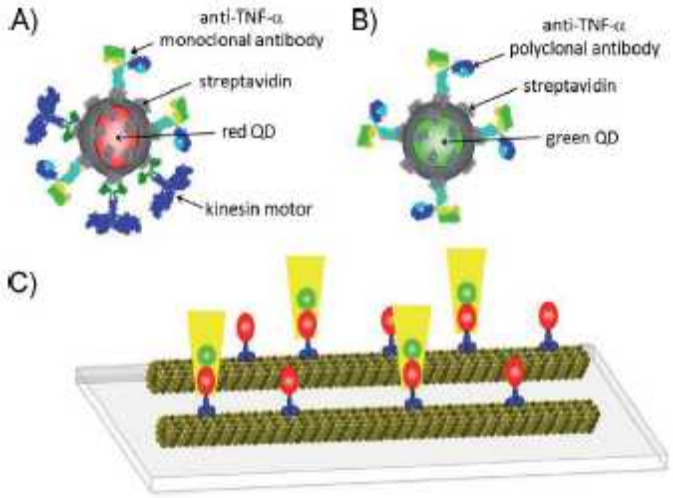
D. Laroche, G. Gervais, M. P. Lilly and J. L. Reno, Nature Nanotechnology 6, 793 (2011).

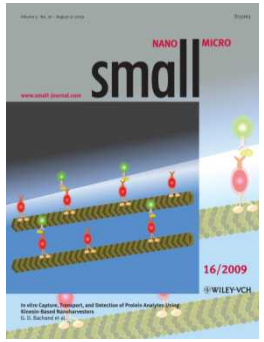
Nanostructured Macromolecular Materials and Assemblies





Bachand & Bachand, *Nanoscale,* 2012, 4, 3706;
Tucker et al., *Small*, 2009, 5, 1279





Carroll-Portillo et al., *Small,* 2009, 5, 1835
Carroll-Portillo et al., *Biotechnol. Bioeng.,* 2009, 104, 1182

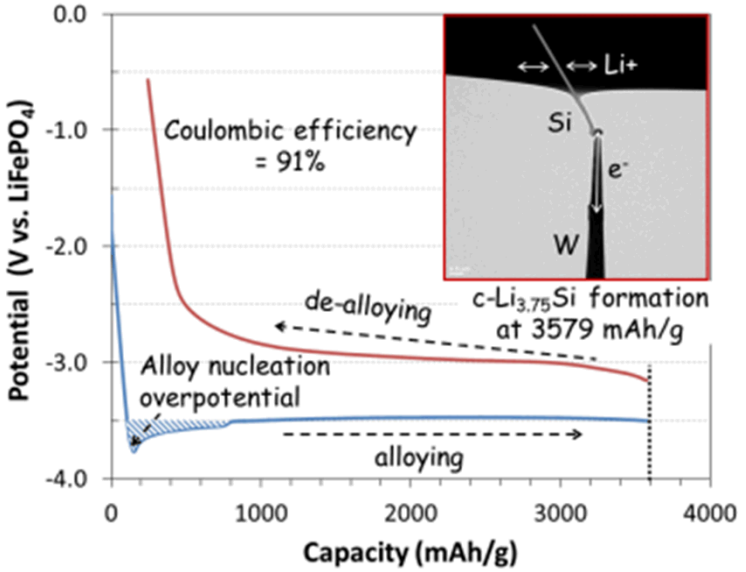
Partnerships with ANL, PNNL, LBNL, SLAC, and numerous universities and industry

Sandia National Laboratories

- JCESR: Joint Center for Energy Storage Research ("the battery hub")
- Methods and instrumentation for precision electrochemistry funded under **the *Nanometer Scale Surface & Interface Phenomena*** project have enabled the study of single electroactive nanostructures

JCESR

Provides the quantitative electrochemistry required for successful electrochemical TEM



130 femtogram of Si undergoing controlled rate alloying with Li

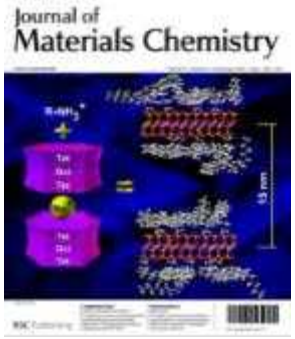
BES--Geoscience

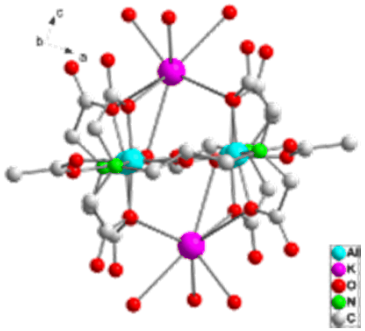
Sandia National Laboratories

Intersection Between the Earth & Engineered Environments

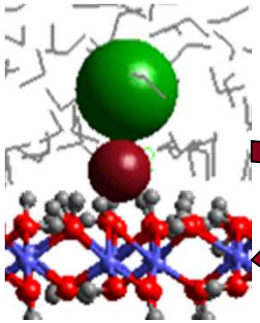
...through research and development in geosciences and sub-surface technologies

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+}

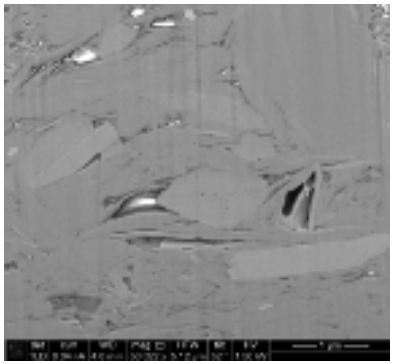
SFG
MM

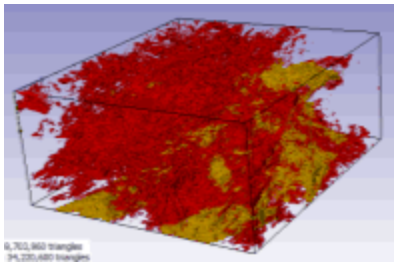
XAS
MM

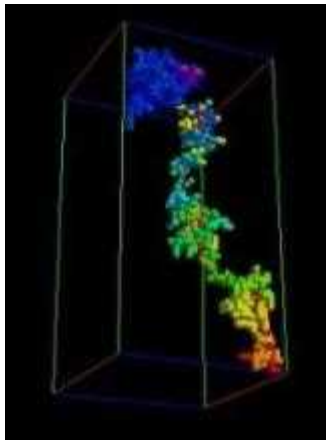
Goethite (FeOOH)

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

3D Pore Networks and Topology





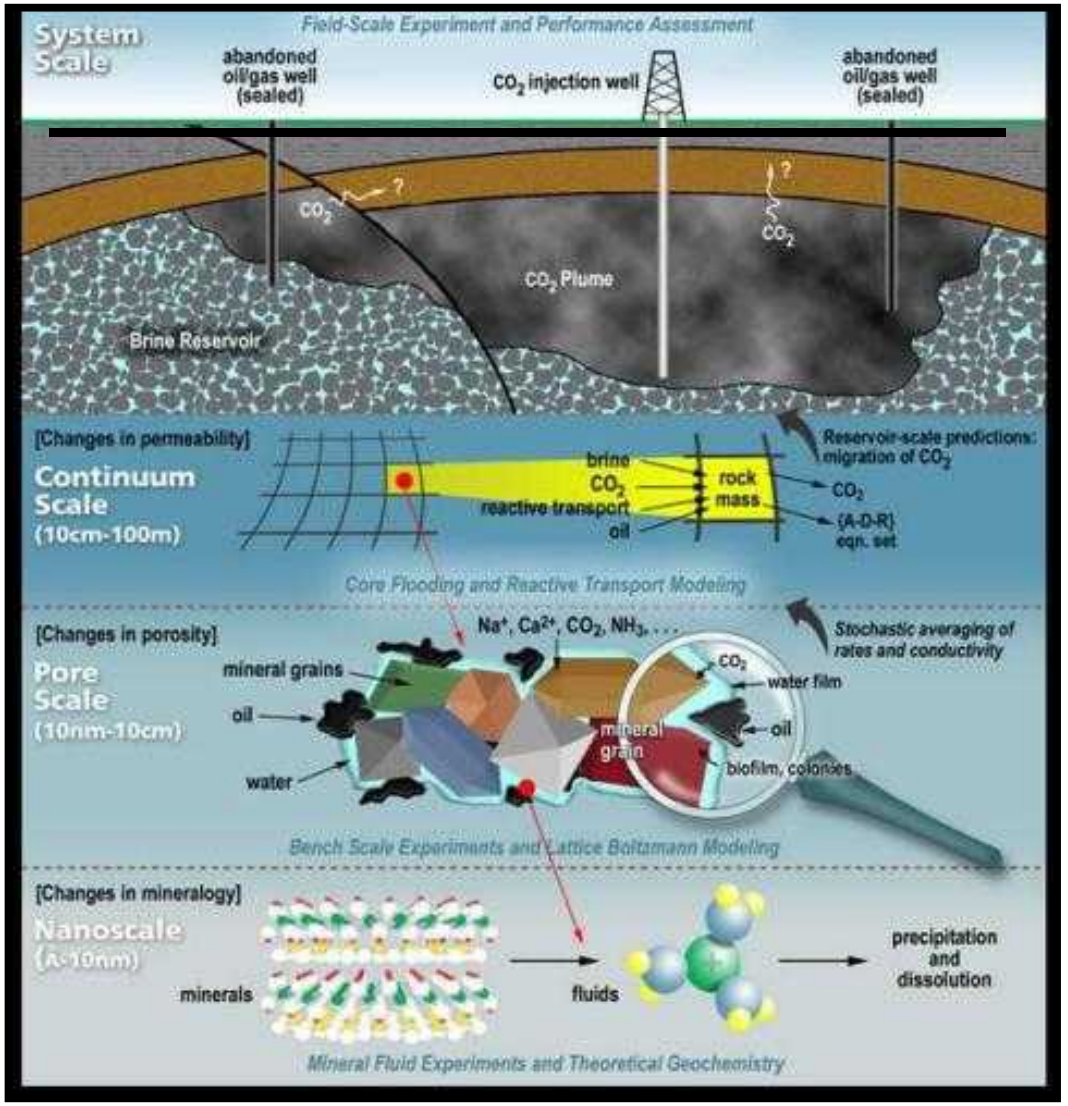


3D invasion percolation model of a displacing liquid invading pores under capillary pressure. Color indicates relative order of pore-filling (Sandia PERC++ software)

Center for Frontiers of Subsurface Energy Security – EFRC

Sandia National Laboratories

Pursuing scientific understanding of multi-scale, multi-physics processes to ensure safe and economically feasible storage of carbon dioxide and other byproducts of energy production without harming the environment.



TEXAS

Sandia National Laboratories

CFSES

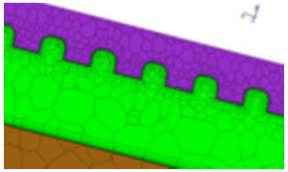
Fusion Energy Science

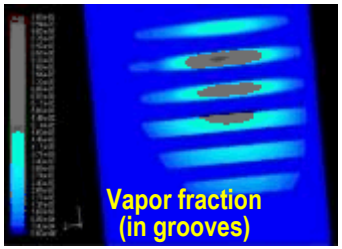
Sandia National Laboratories

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

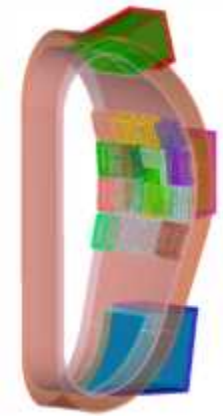
Thermal-hydraulic analysis

Coolant flow and heat transfer reference calculations for ITER.

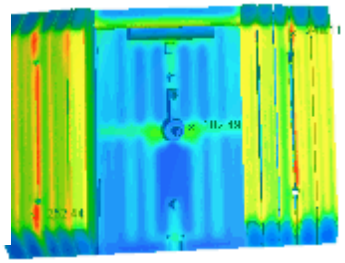




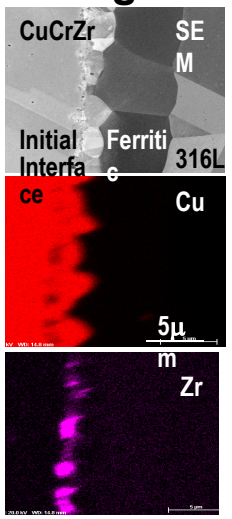
Hypervaportron model (FLUENT) of ITER first wall

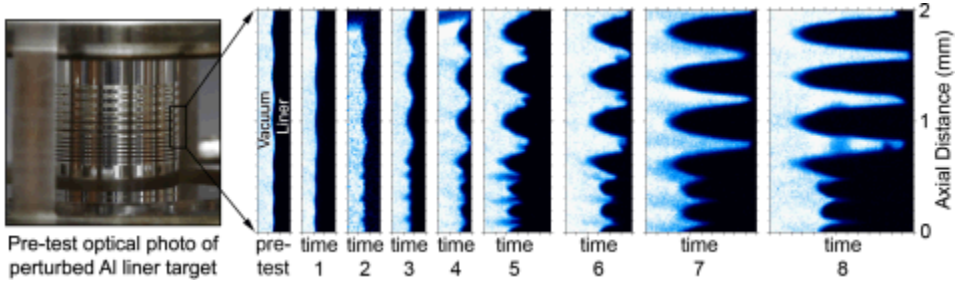


Thermal & stress analyses



Joining R&D





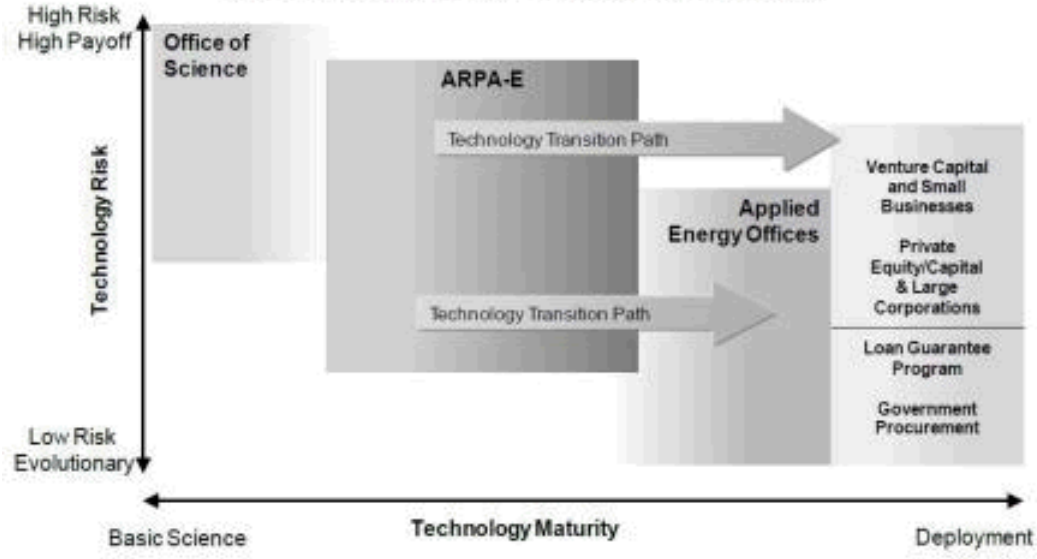
Pre-test optical photo of perturbed Al liner target

Fundamental Instability Measurements in Magnetically Driven Z-Pinch Liner Implosions: Precision radiography.

ARPA-E

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

Figure: ARPA-E Coordination within DOE and with Other Stakeholders



Example project areas:

Improved power grid system operations using advanced stochastic optimization
High precision tester for automotive and stationary batteries
Silicase weathering
Agile power converter for PV applications - Utilizing advanced wide-bandgap devices

Energy & Climate Laboratory-Directed Research and Development

Sandia National Laboratories

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

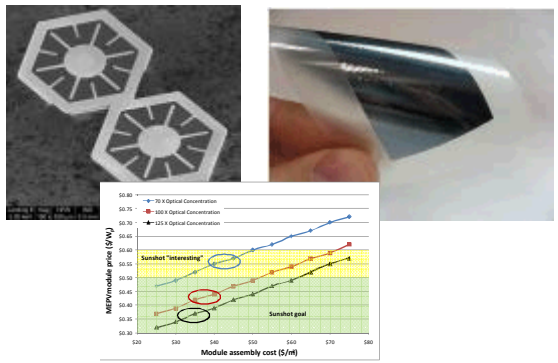
Develop and support SMU-needed capabilities through targeted Laboratory-Directed Research & Development (LDRD) projects.

Twistact Technology

Demonstrated monolithic endless belts using cold pressure welding

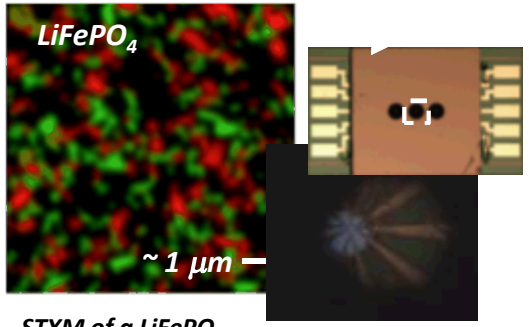
Microsystems- Enabled Photovoltaics

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