Electronic and Optical Materials Science and Engineering at Sandia National Laboratories

SAND2019-13938PE

Presented by

Ryan P. Haggerty, PhD

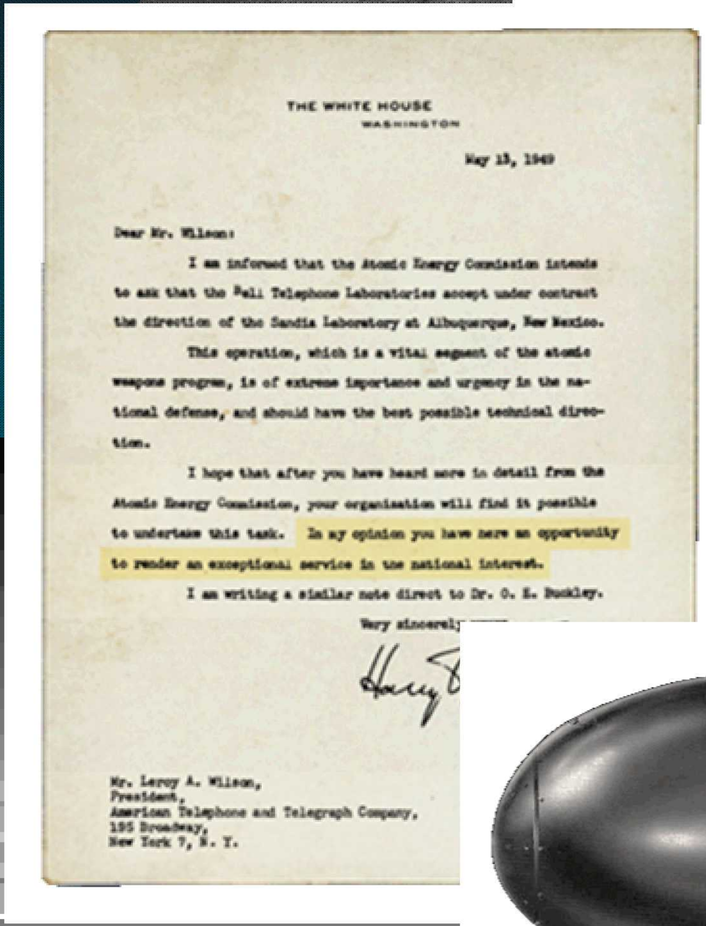
R&D Manager
Electronic, Optical & Nano Materials
Material, Physical and Chemical Science Center

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SANDIA'S HISTORY IS TRACED TO THE MANHATTAN PROJECT

…In my opinion you have here an opportunity to render an exceptional service in the national interest.

- July 1945
  Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949
  Sandia Laboratory established
- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–2017
- Honeywell: 2017–present



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

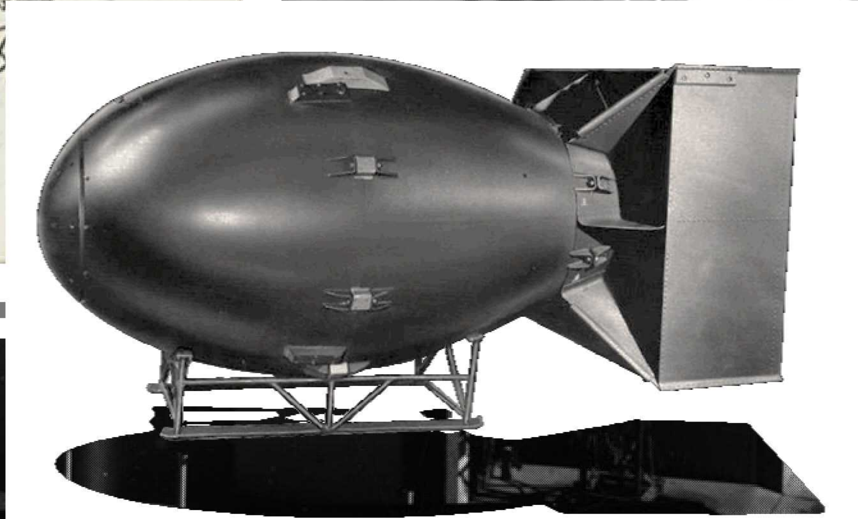
This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely,

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.



SANDIA IS A FEDERALLY FUNDED RESEARCH AND DEVELOPMENT CENTER MANAGED AND OPERATED BY

National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc.: 2017 – present

Government owned, contractor operated

SANDIA HAS FACILITIES ACROSS THE NATION

Activity locations

- Kauai, Hawaii
- Waste Isolation Pilot Plant, Carlsbad, New Mexico
- Pantex Plant, Amarillo, Texas
- Tonopah, Nevada

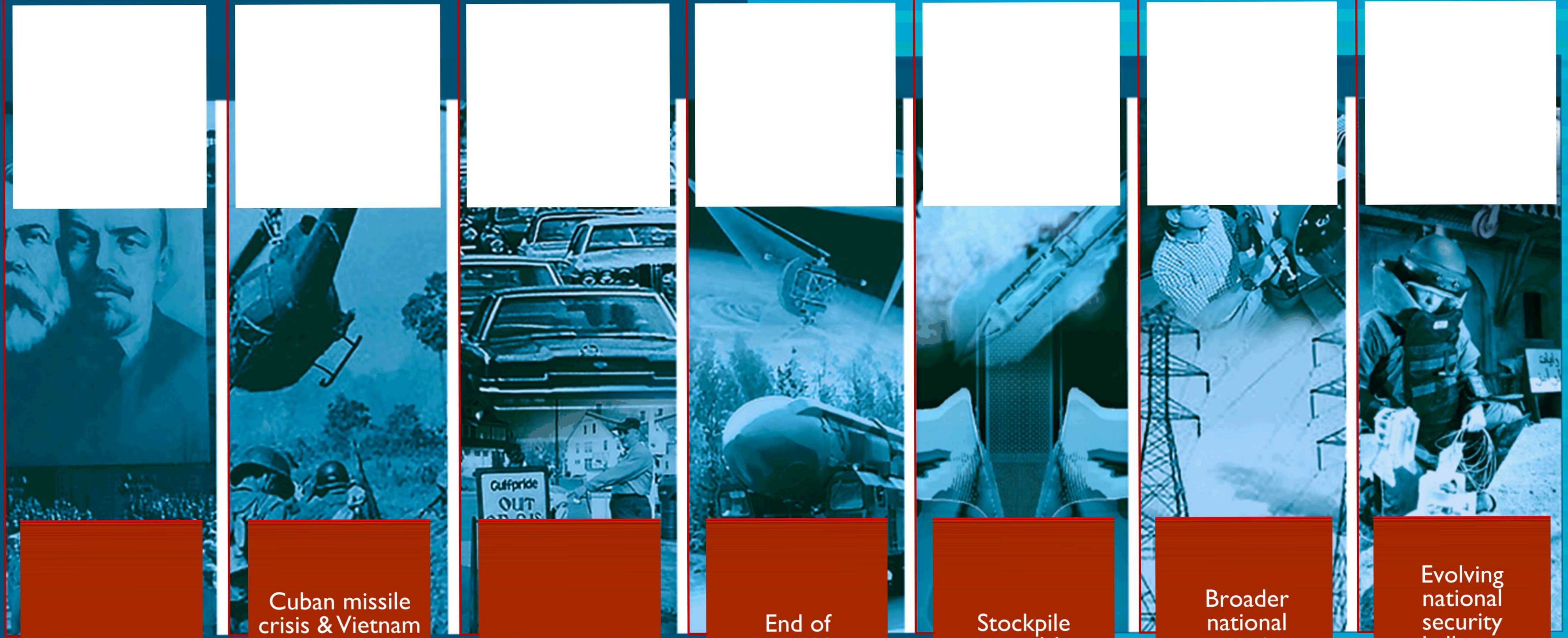
Main sites

- Albuquerque, New Mexico
- Livermore, California

PURPOSE STATEMENT DEFINES WHAT WE DO

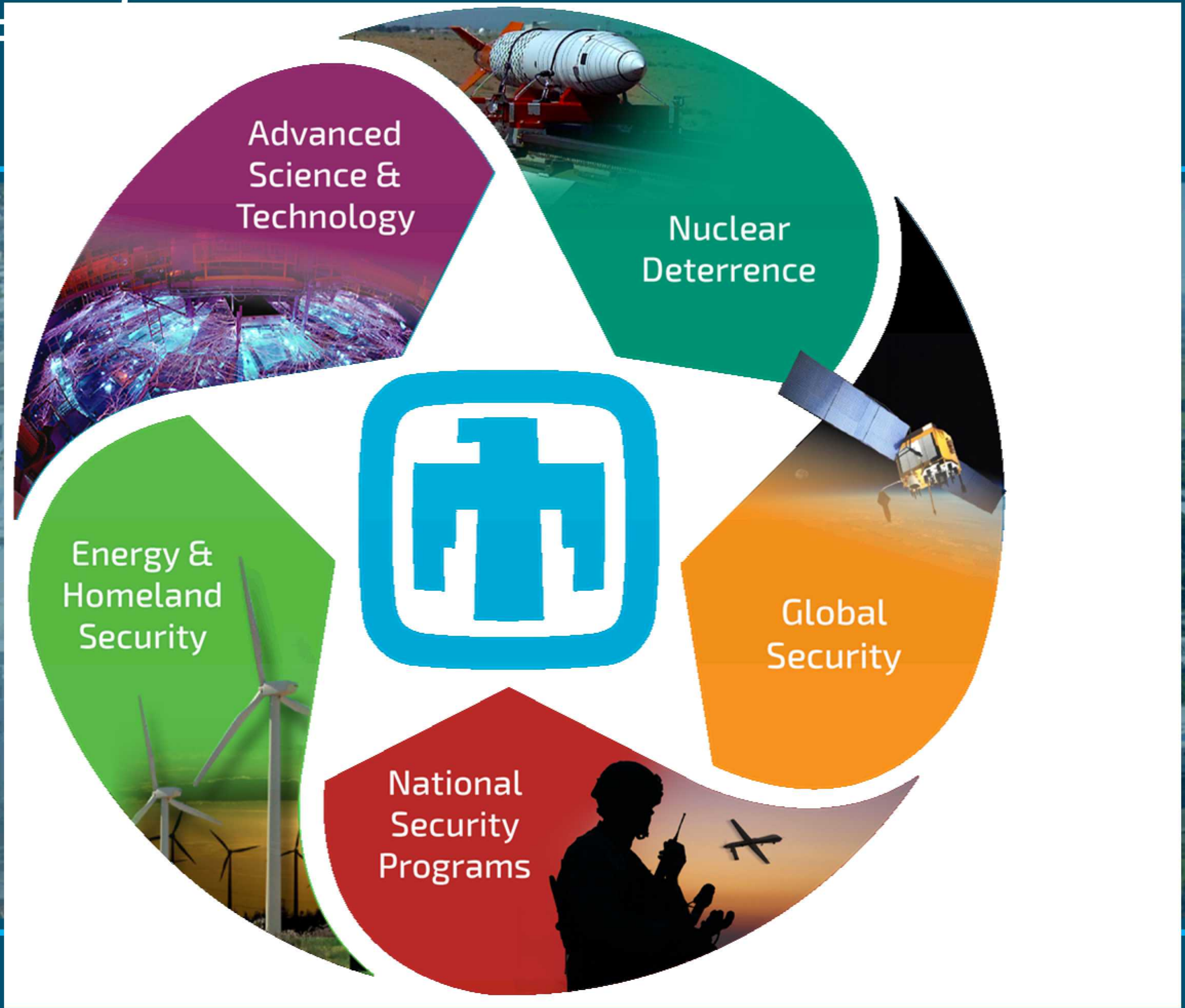
Sandia develops advanced technologies to ensure global peace

SANDIA ADDRESSES NATIONAL SECURITY CHALLENGES



1950s	1960s	1970s	1980s	1990s	2000s	2010s
Arms race	Cuban missile crisis & Vietnam War	Energy crisis	End of Cold War	Stockpile stewardship	Broader national security	Evolving national security challenges

SANDIA HAS FIVE MAJOR PROGRAM PORTF



Sandia Materials & Process Science

- ***Fundamental Materials & Process Science***
  - Develop/integrate theoretical insights, computational simulation tools, and experiments to provide foundational, predictive understanding
  - Develop innovative new materials and process technologies
  - Create advanced materials analysis & process diagnostics tools
- ***Materials & Process Advanced Development***
  - Advanced & exploratory materials & process development
  - Production process development & technology transfer
- ***Materials Engineering/Production Support***
  - Materials & process selection/optimization
  - Problem solving, production support
  - Understanding & quantifying the margins

Multiple Large Materials R&D Facilities

Processing & Environmental Technology Laboratory

Center for Integrated Nano Technologies

Thermal Spray Research Laboratory

Advanced Materials & Processes Laboratory

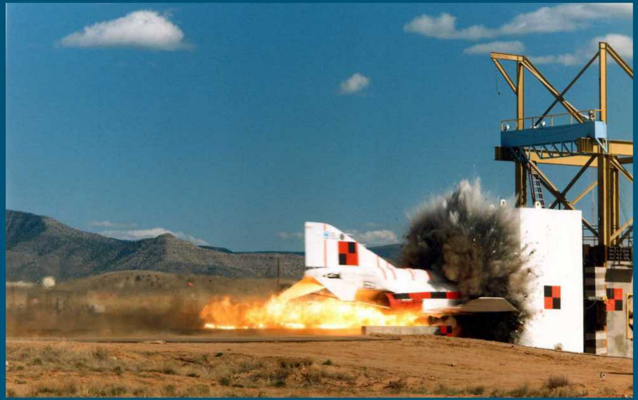
Ion Beam Laboratory

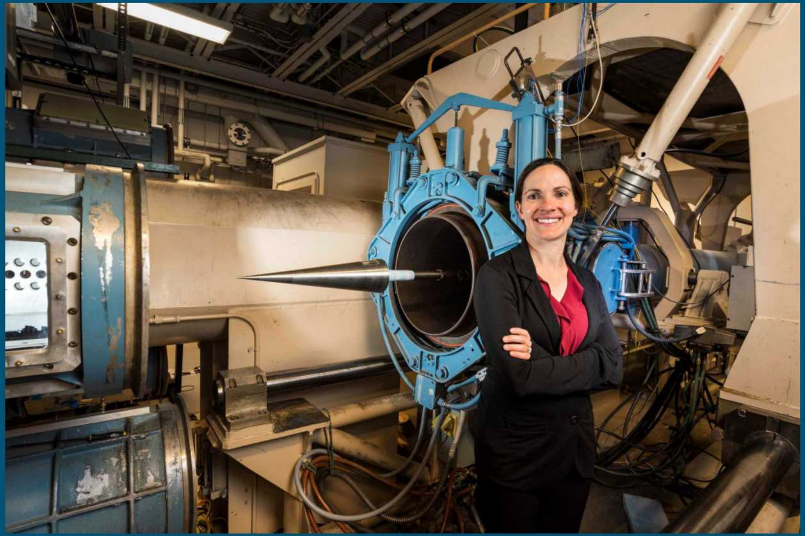
Integrated Materials Research Laboratory

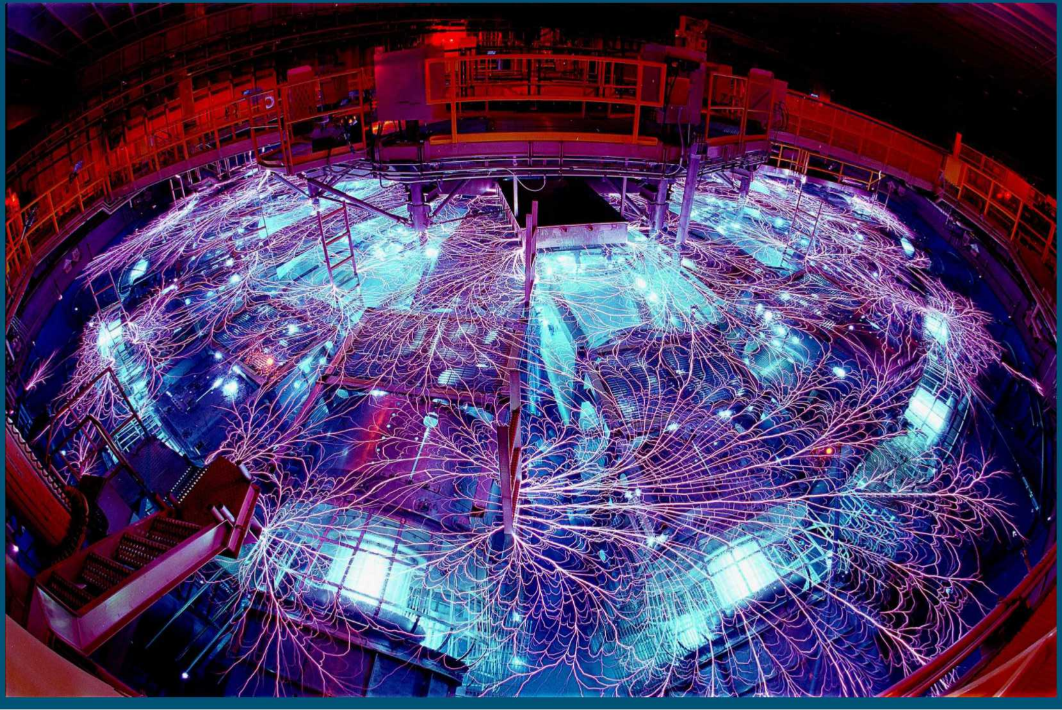
Microsystems Science & Technology Center

Advanced Materials Laboratory

Large Scale Testing at Sandia



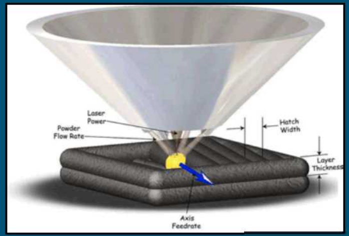


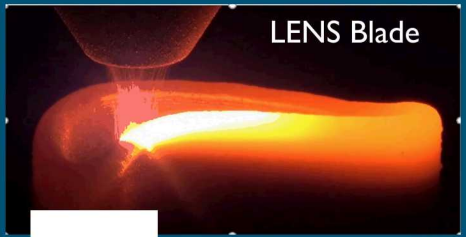

30+ Years of Sandia AM Technology Development & Commercialization

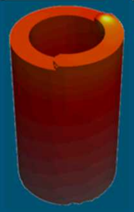
FastCast *

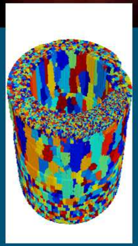
Development Housing

Laser Engineered Net Shaping LENS®



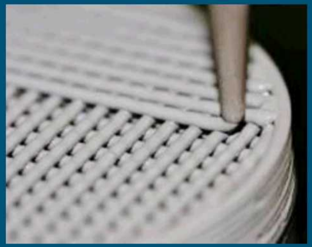


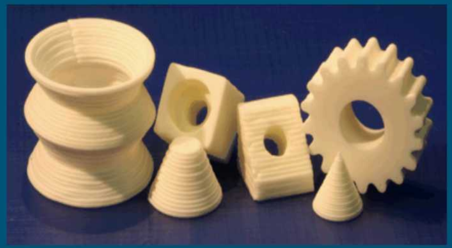




Grain morphology prediction

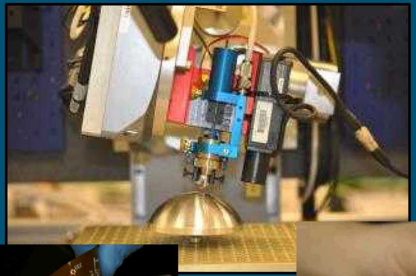
Robocasting *

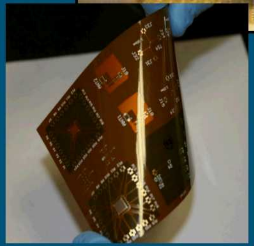




Ceramic, energetics, elastomers

Direct Write

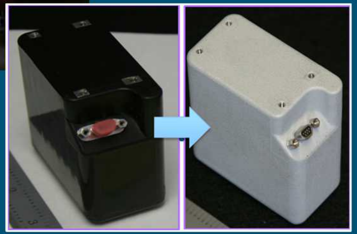




Conformal Printing, flexible electronics, power sources

Thermal Spray

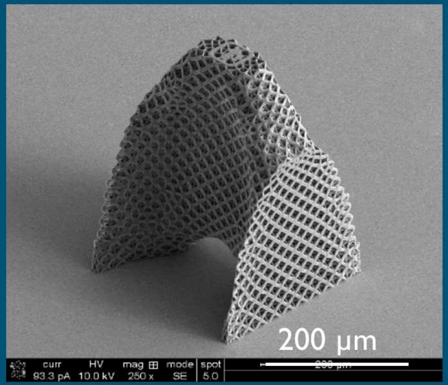
Spray-formed Rocket Nozzle



Metal on Plastic

Micro-Nano Scale AM

Lattice Structure



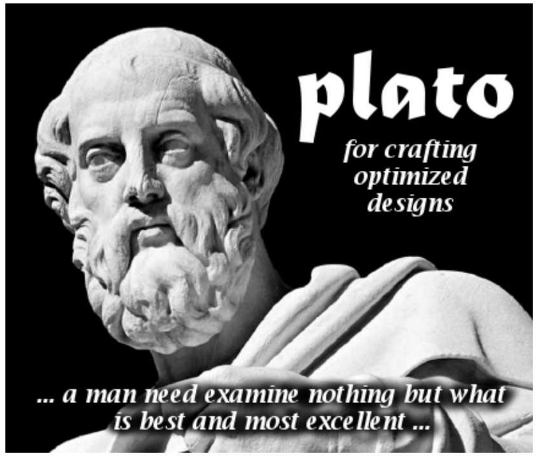
* = Licensed/Commercialized Sandia AM technologies

Underline = Current Capability/Activity

High Operational Tempo (HOT SHOT)

A sounding rocket designed and launched by Sandia lifts off from the Kauai Test Facility in Hawaii on April 24. (Photo by Mike Bejarano and Mark Olona, Sandia Lab News)

PLATO Design Platform



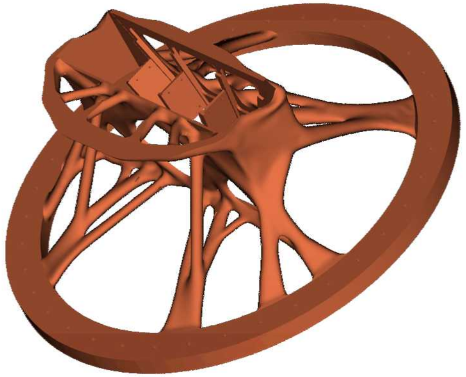
End-user environment for physics-based design using topology optimization

HPC-enabled: physics, optimizers, services, …

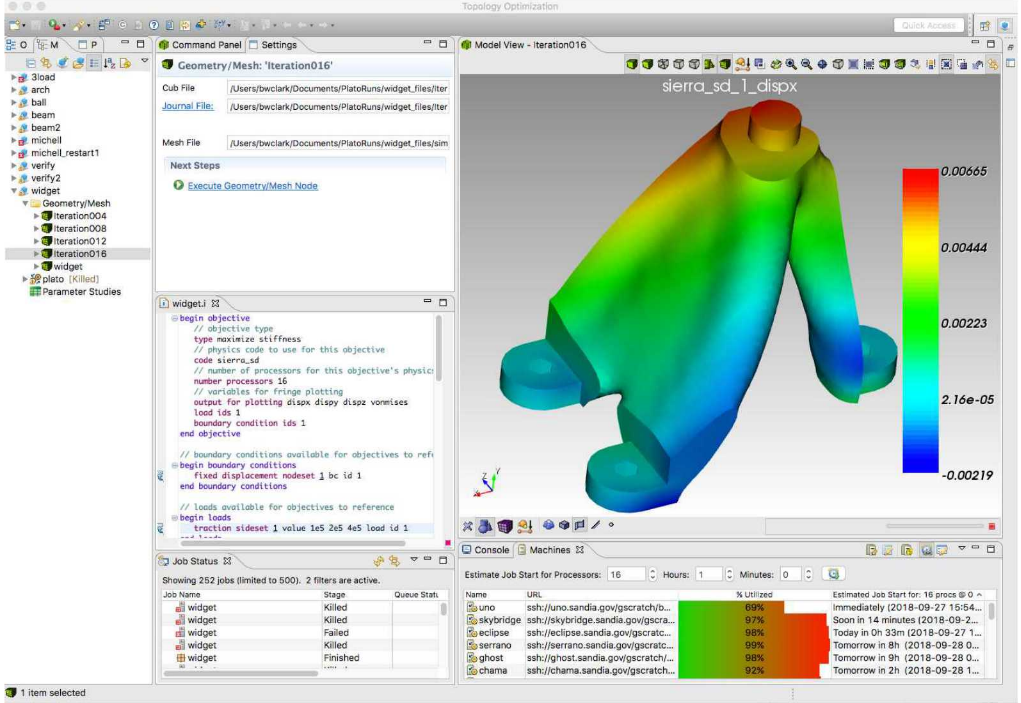
Interactive design feedback and user control

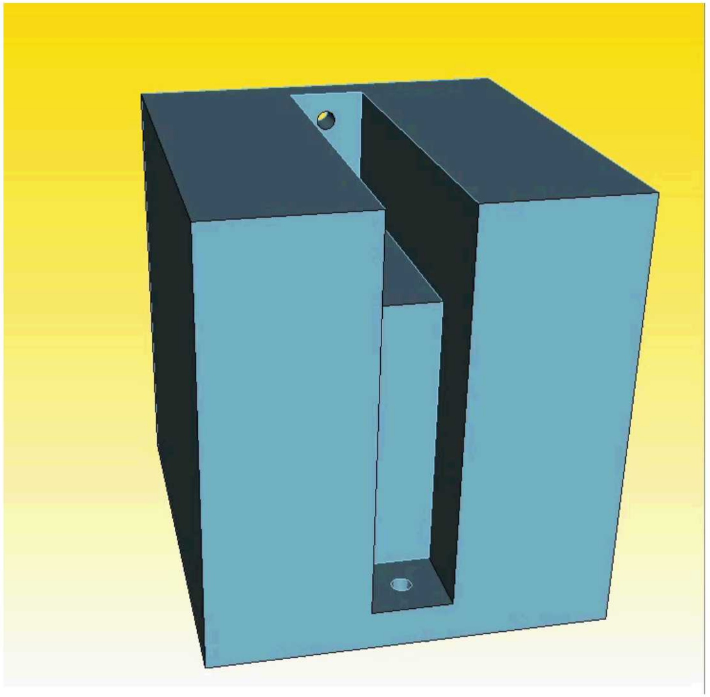
Smooth, print-ready designs

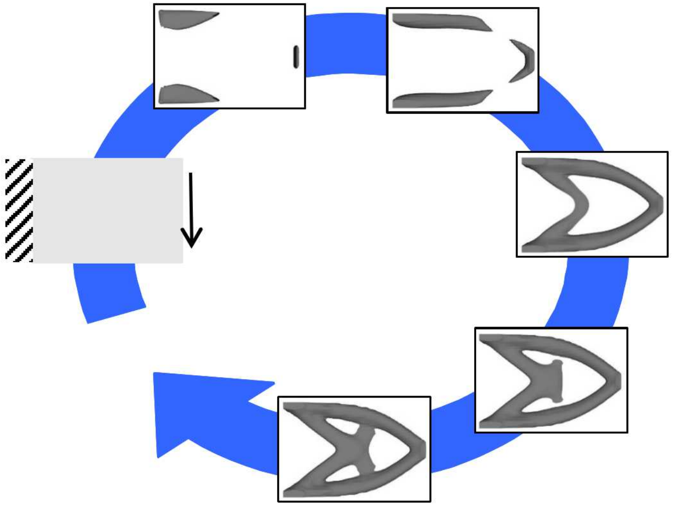
Extensible architecture



Website: www.sandia.gov/plato3D
Github: https://github.com/platoengine/platoengine
email: plato3D-help@sandia.gov







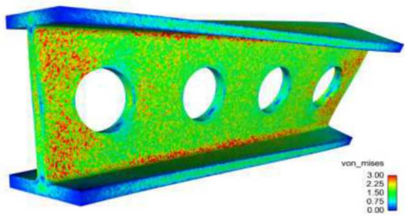
Interactive design feedback and user control

Brett Clark, Josh Robbins, Miguel Aguilo

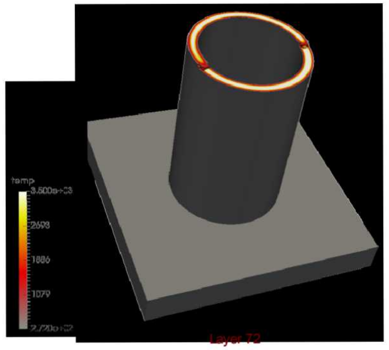
Qualification Tomorrow

"Changing the Engineering Design & Qualification Paradigm"

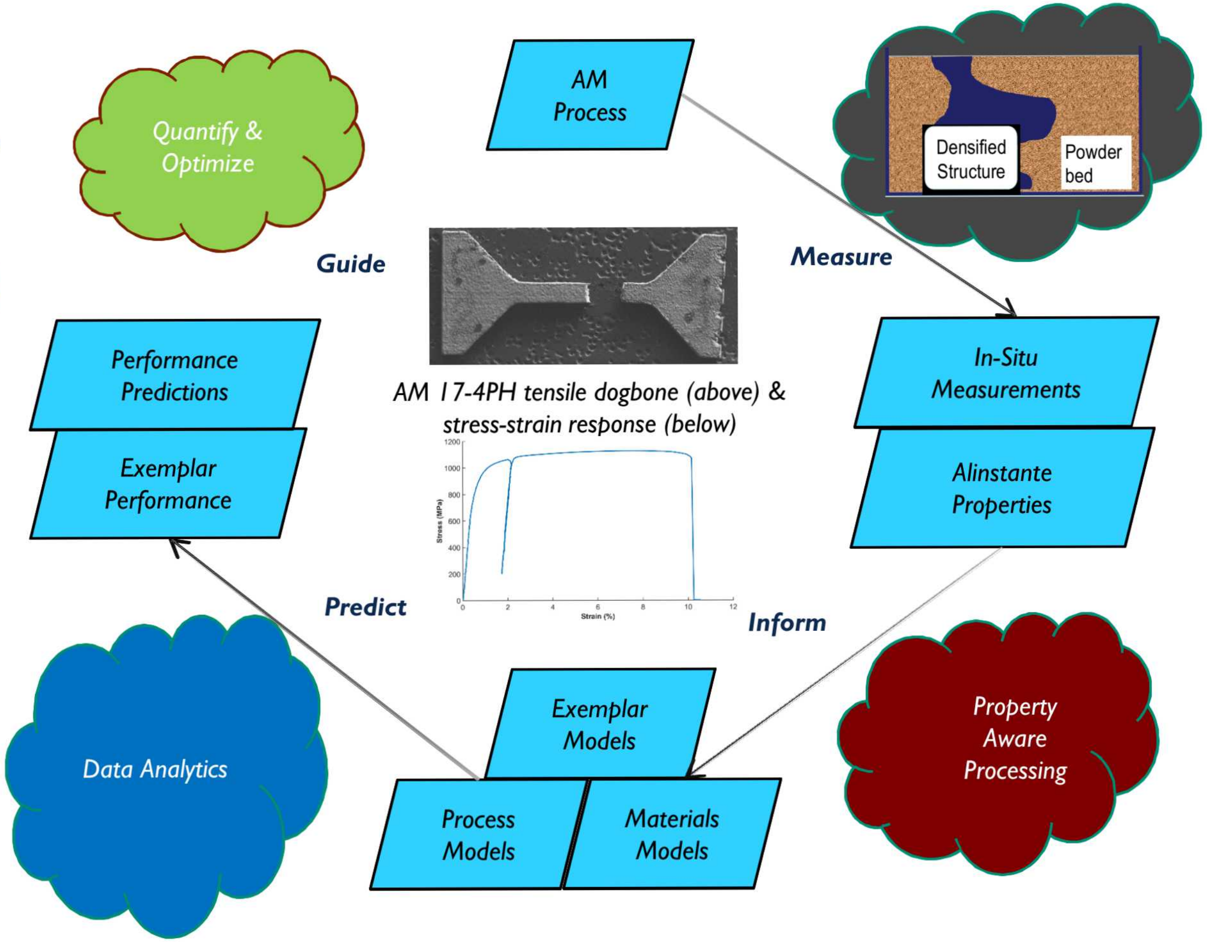
- leverage AM, in-process metrology & HPC to revolutionize product realization
- accelerating design to production

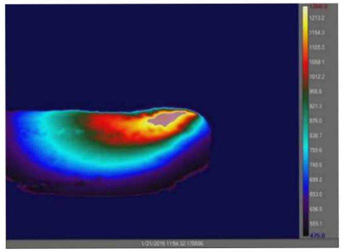


material / part performance simulation

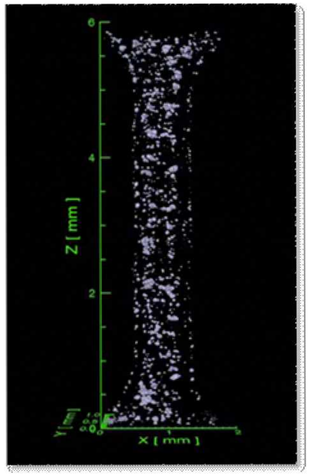


process simulation





thermal history during bi-directional metal deposition



17-4PH dogbone porosity

*Roach, **SFF Proceed.**, 2018*

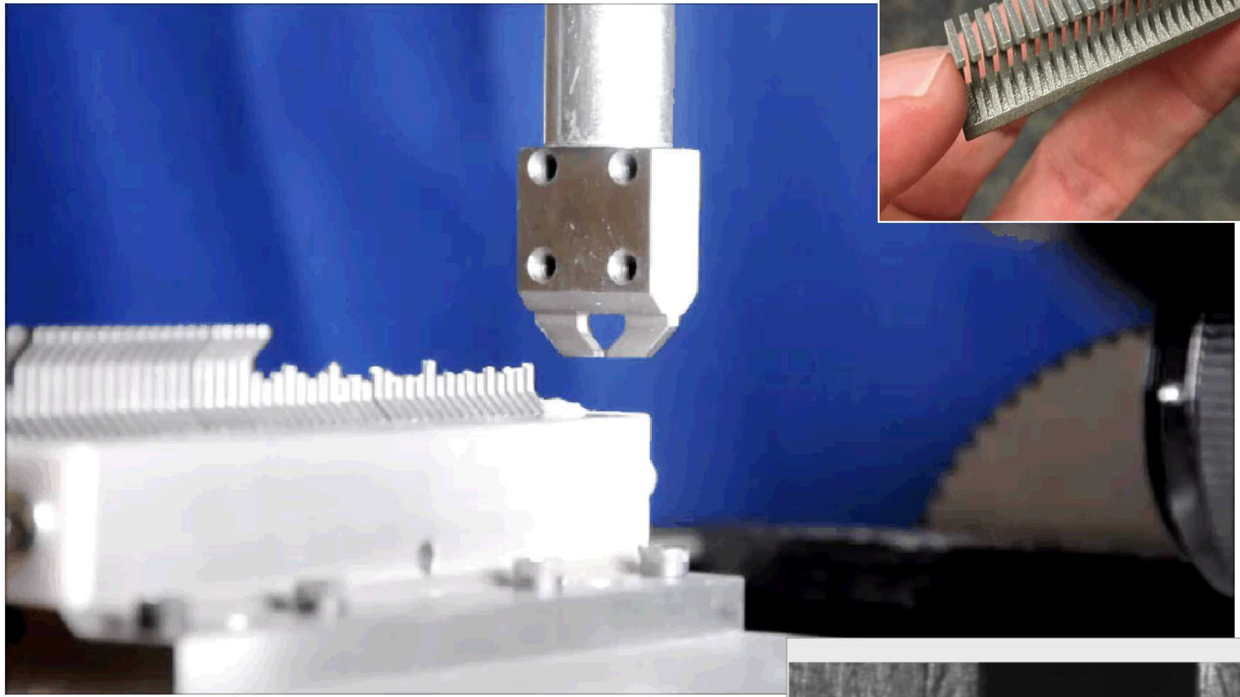
High Throughput Testing - Alinstante

Properties… In an instant
- printing is fast
  - hundreds of samples in days
- test/measurement is common constraint

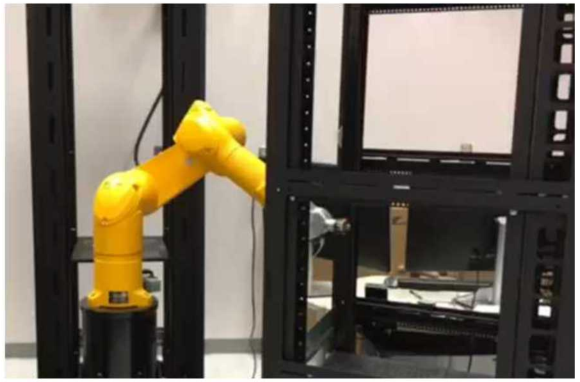
Need automation & robotics
- consistent, rapid, & efficient

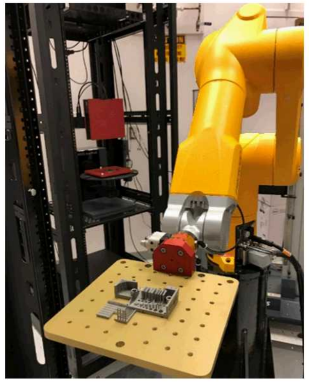
Alinstante wish list:

Properties	**Structure**	**Process**
Tensile strength	Geometry	Surface remediation
Ductility	Roughness	Heat treatment
Toughness	Porosity	Subtractive machining
Hardness	Chemistry	Coating
Wear & friction	Phase content	Joining
Permeability	Grain Size	Integration
Thermal expansion	Crystal Texture	etc.
Reactivity/corrosion	Residual stress	
Electrical conductivity	Dislocation content	
Resonance	etc.	
etc.		

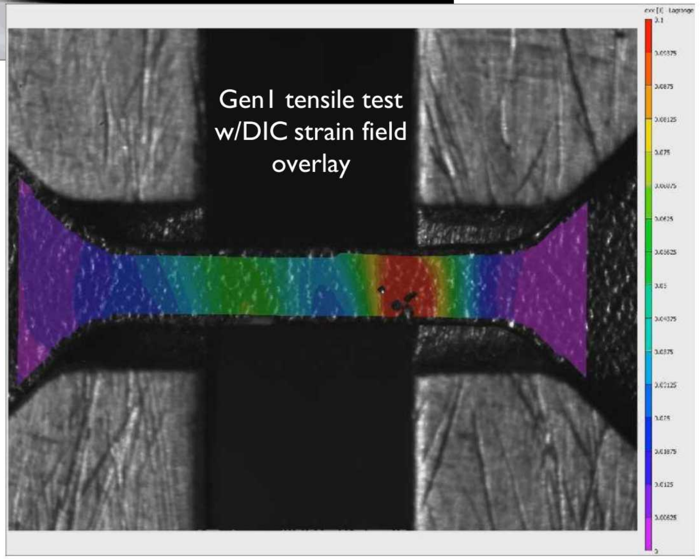


*Heckman, **Mat. Sci. Eng. A**, submitted*





robotic work cell for material characterization



Electronic, Optical and Nano Materials Department

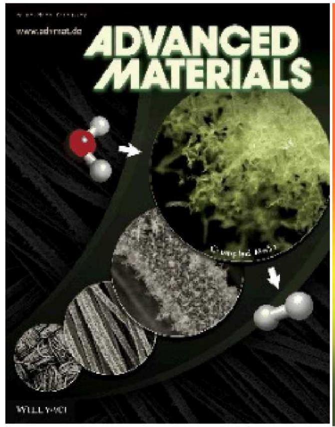
Electronic, Optical and Nano Materials Department

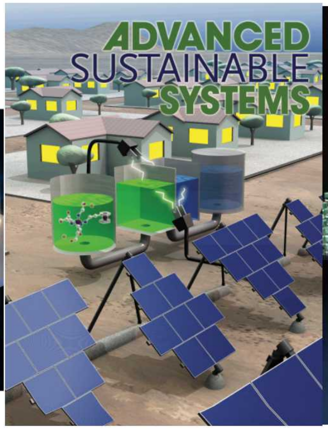
Mission

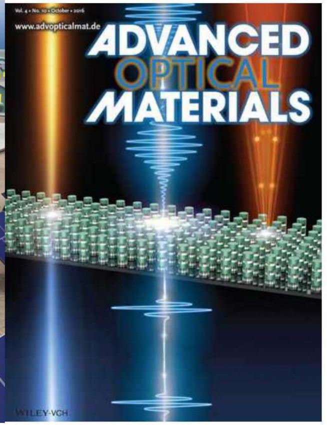
Materials innovation to enable novel engineering and disrupt current nuclear weapons and defense technologies.

How we do it

We develop new material and new applications of existing materials with novel electrical and optical properties, utilizing a physics based understanding of electromagnetic interactions and ionic transport at all length scales, molecular, crystallographic, microstructural and in bulk materials.





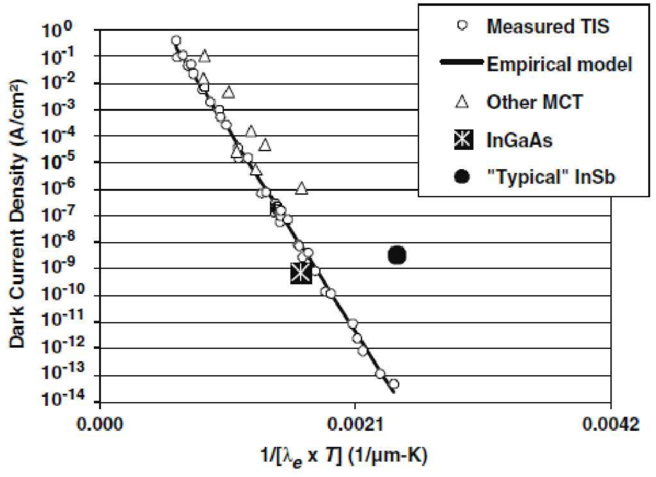


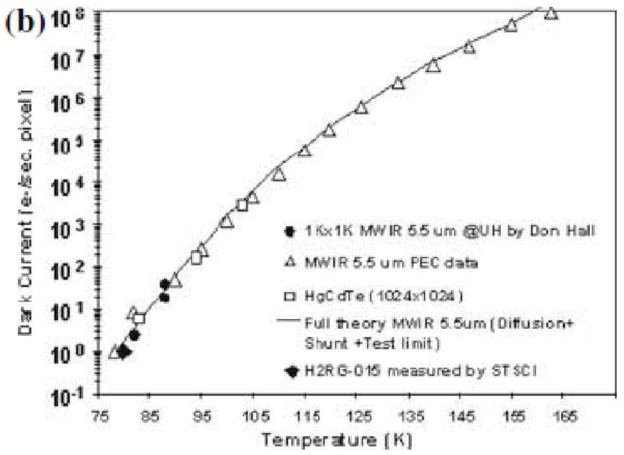
Core Areas:
- Dielectric breakdown
- Electronic Ceramics (e.g. Ferroelectrics)
- Metamaterials (optical and acoustic)
- Scintillators
- Microscale processing
- Ceramics processing

Improving Infrared Sensing Using Nanoantennas

Infrared Sensing Today

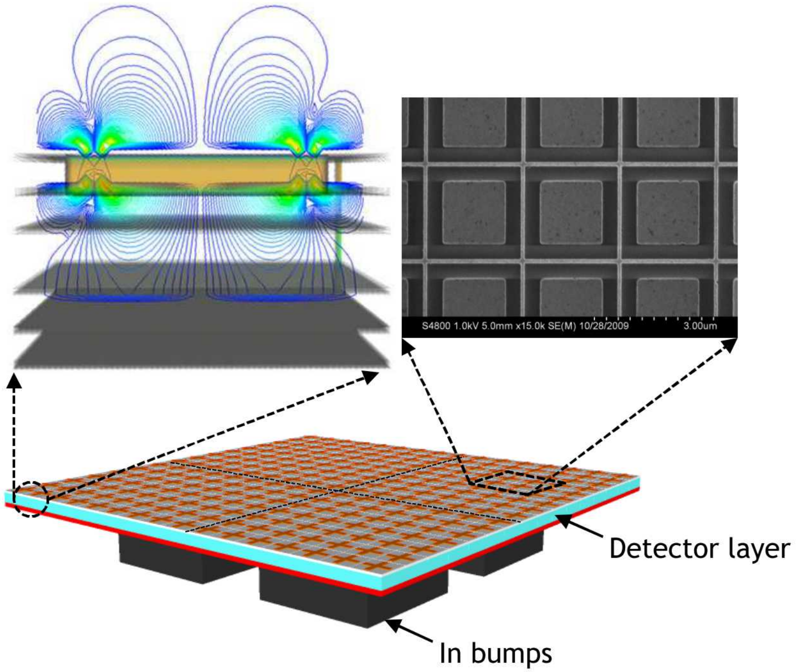
- Industry is dominated by mercury cadmium telluride (MCT) focal plane arrays.
  - This material is very well established.
  - It has limitations in processing and dark current.
- Other materials are much earlier in maturity, but could have advantages in dark current.
  - Superlattice designs in III-V materials are an example.
  - Have lower absorption than MCT, requiring thick layers.
- Thickness normally determined by absorption coefficient of the detector material.
  - Thick layers result in higher dark current and incomplete carrier extraction due to short carrier lifetime.



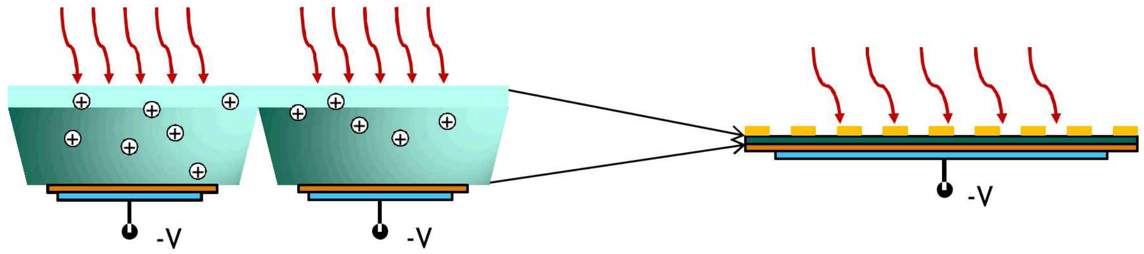


Tennant, W., et al., *J. of Electronic Materials*, **37**, 2008.
Tennant, W., *J. of Electronic Materials*, **39**, 2010.

Change the Architecture



- Use a nanoantenna (metasurface) to convert incoming radiation to a mode with energy confined to a small volume.
- Allows us to use thin layers of detector material.
  - Low dark current, low crosstalk, full carrier extraction for high EQE
- This confinement is what enables us to look at new concepts.
  - Voltage tunable materials
- The pattern may be changed from pixel-to-pixel allowing adjacent pixels to have different spectral or polarization response.



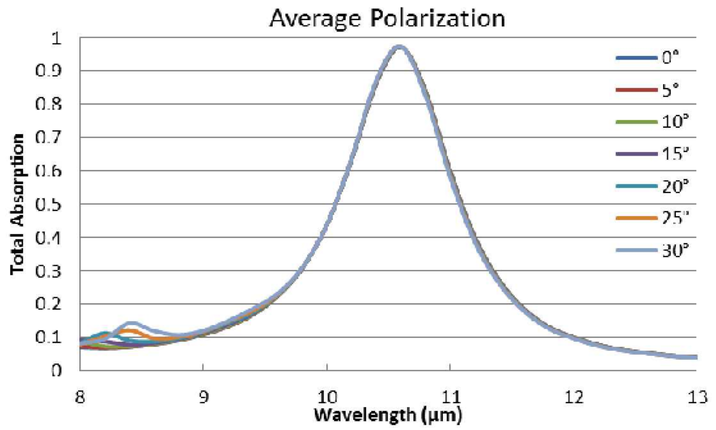
Dark Current $J_{Diff} = \frac{e \cdot n_i^2 \cdot t_{abs}}{N_D \cdot \tau_p}$

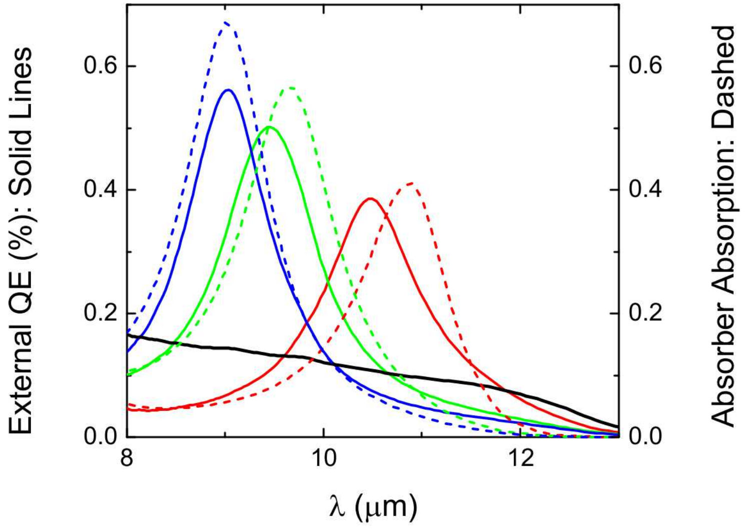
U.S. Patents: 8,452,134, 8,750,653, and 8,897,609

Nanoantenna Optical Properties

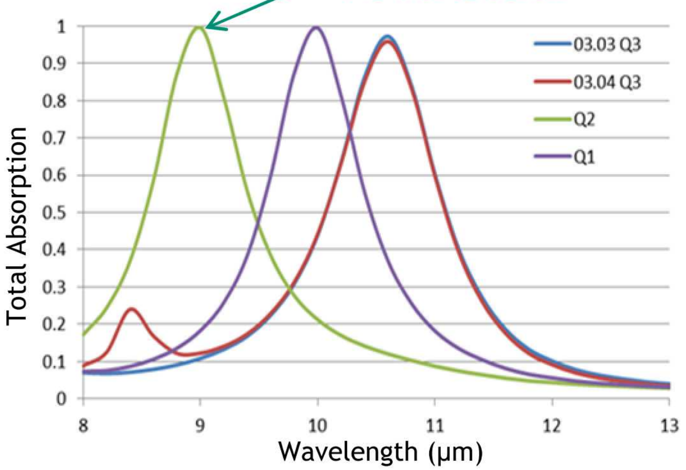
- The nanoantenna couples the incoming light to a confined mode with no reflection at the design wavelength.
  - Achieved with a single patterned metal layer.
  - No AR dielectric stack required
- The AR effect does not change with angle as it would with a dielectric AR coat.
- Polarization independence over angular range of interest.
- Increase in EQE over bare material.

Angular Insensitivity





No reflection

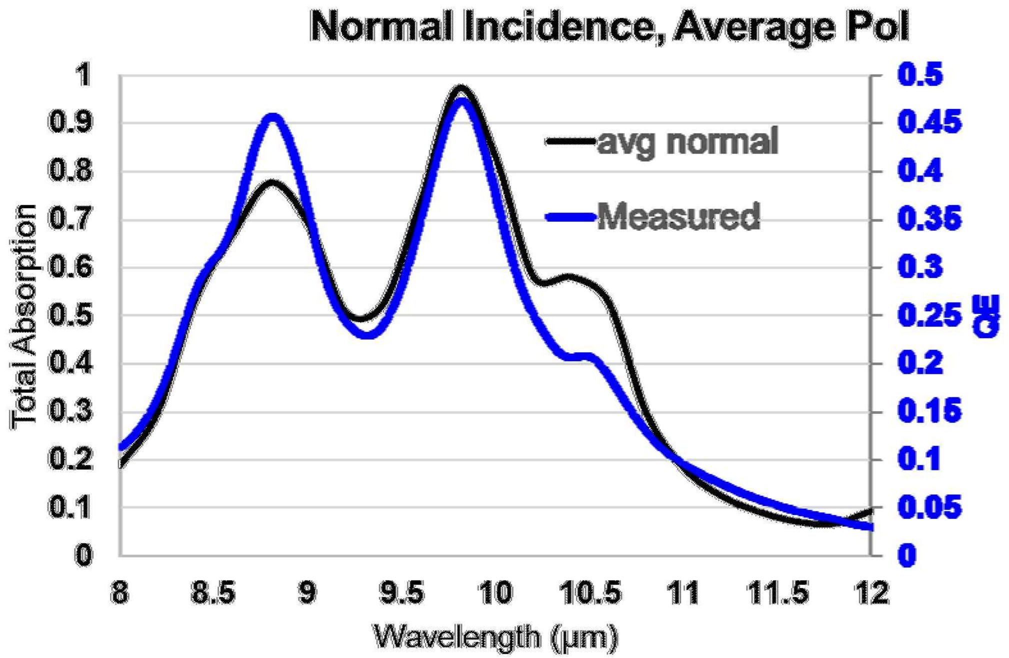


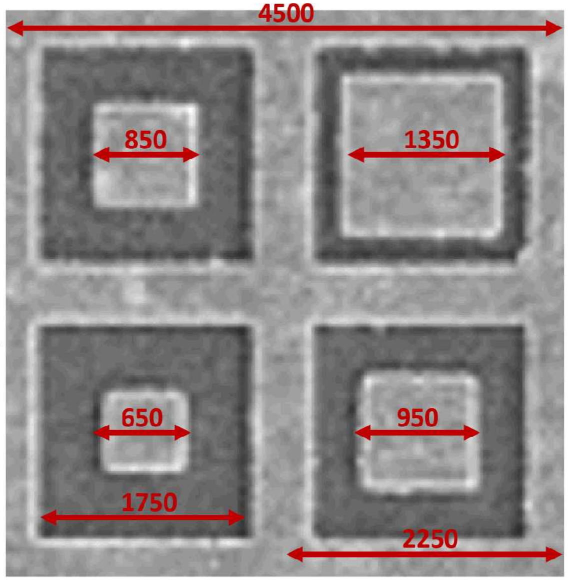
Tailoring Spectral Bandwidth

Spectral bandwidth increases by 2x

Flat-top response possible by better tuning NA

Can tailor a passband to user needs

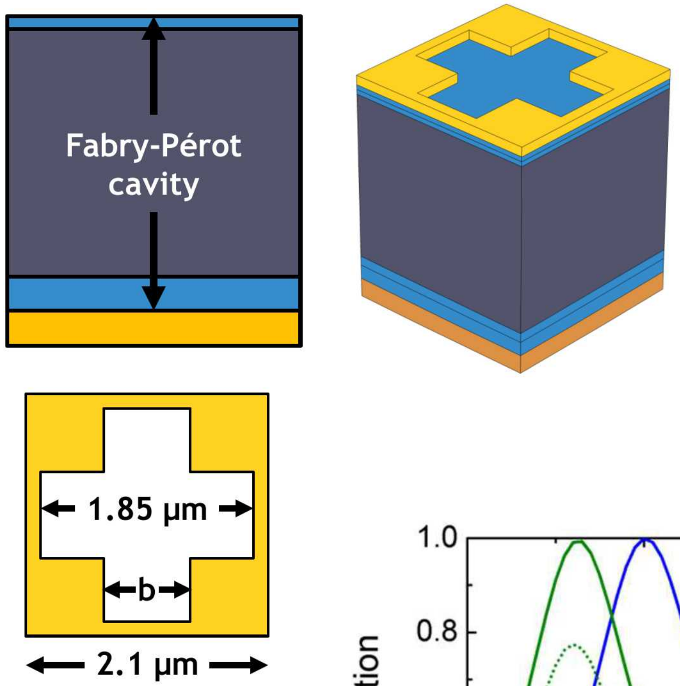




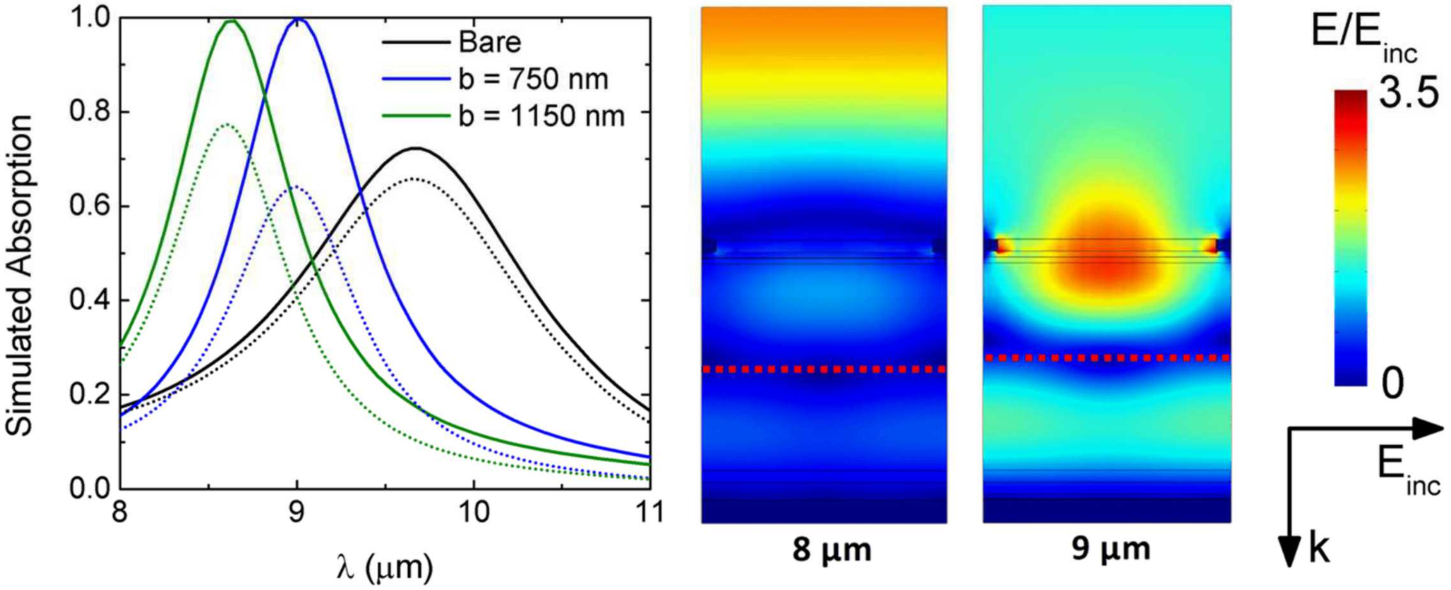
nanometers

M.D. Goldflam, *et al.*, "Next-generation infrared focal plane arrays for high-responsivity low-noise applications," IEEE Aerospace Conference, Mar. 2017.

Modeling: Nanoantenna-Enhanced Detector



- Employ two coupled resonances: Fabry-Pérot cavity with metal nanoantenna.
- Variable response in fixed detector through variation of nanoantenna only.
- Can be polarization independent or polarization sensitive.

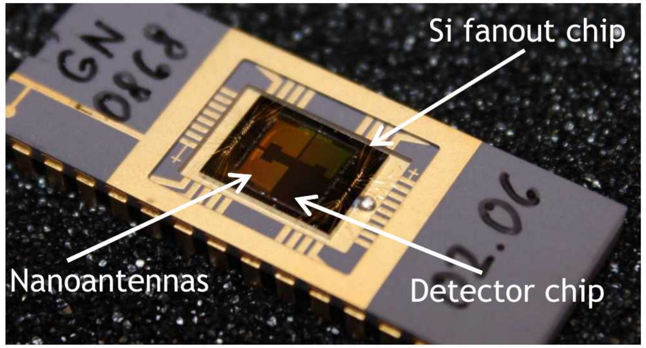


Comparison to Experimental Results

Demonstrated NA-thinned superlattice photodetector for the first time

- 2 to 3x higher QE than conventional SL photodetectors
- Similar dark current to conventional SL photodetector of same thickness

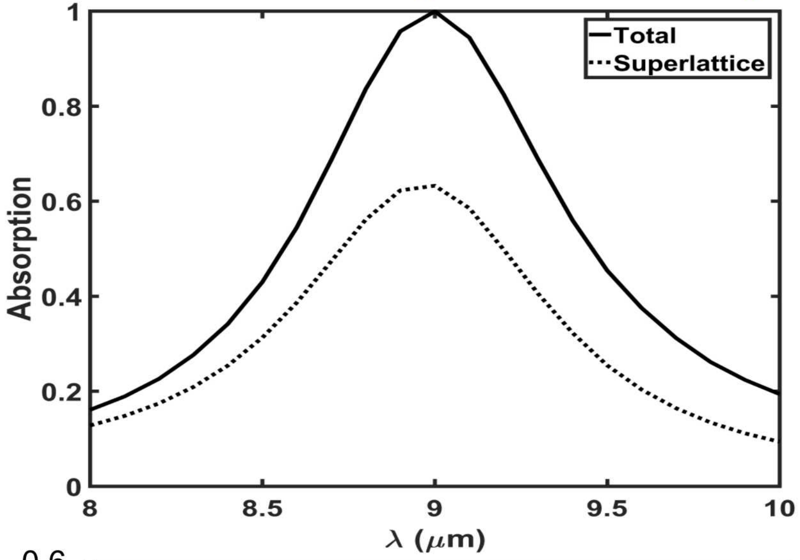
Good agreement between measured EQE and simulated absorption in detector layer.

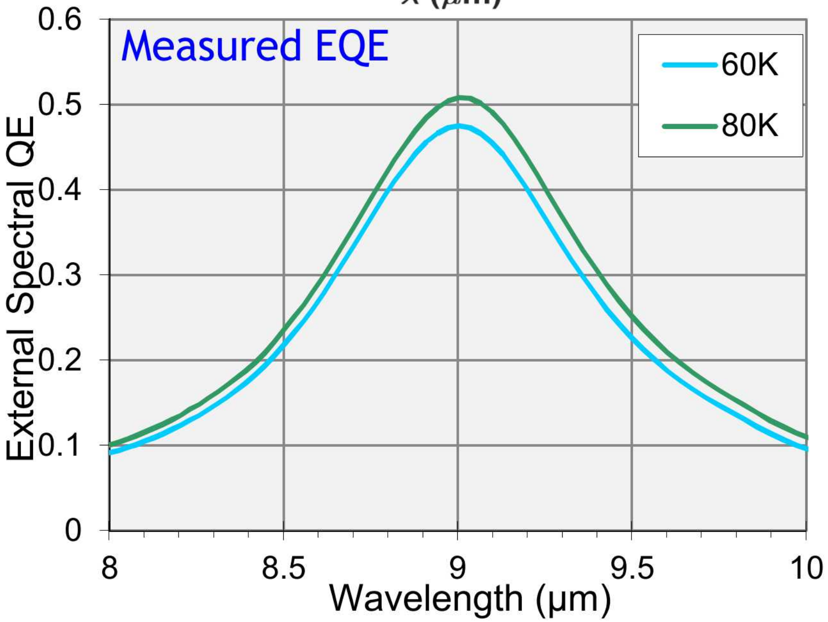


Optical losses may be reduced by optimizing the device parameters.

M. D. Goldflam, *et al.*, *Appl. Phys. Lett.*, vol. 109, 251103, Dec. 2016.

Simulation of absorption in active layer

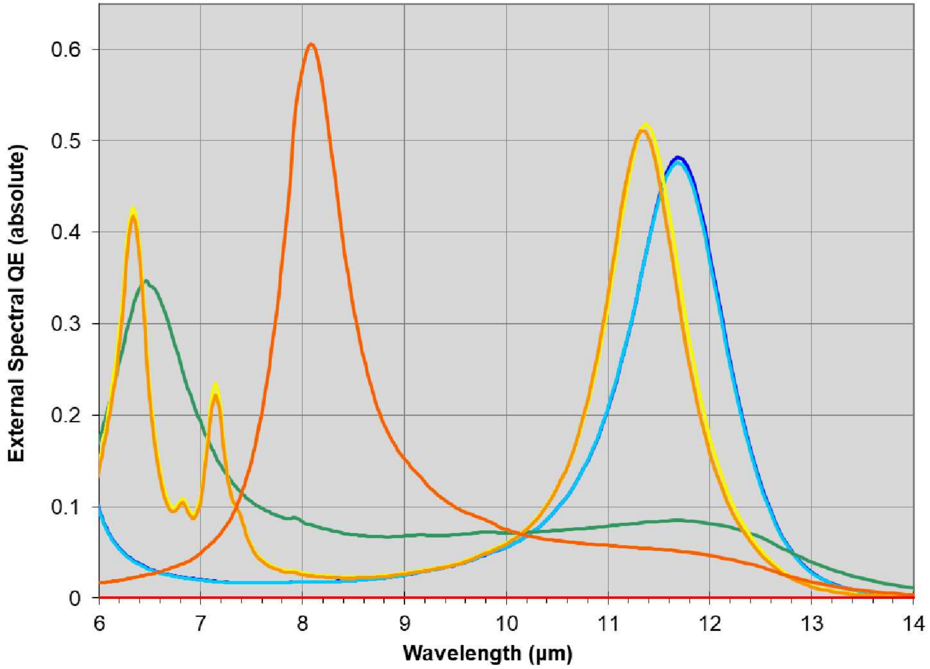




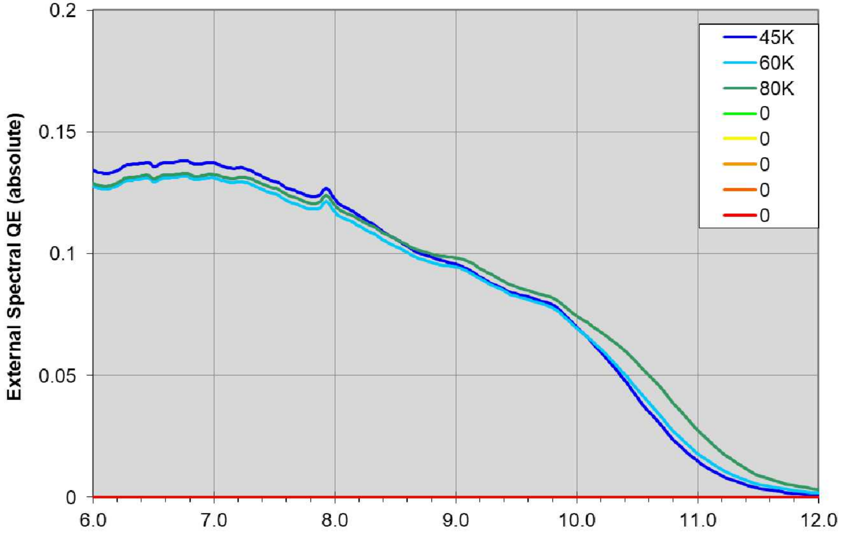
Quantum Efficiency

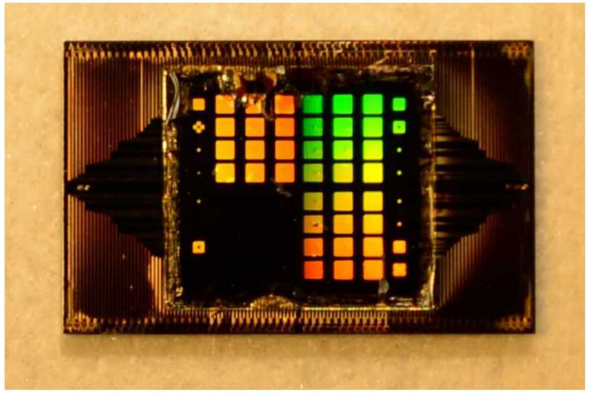
- High external quantum efficiency
  - Achieves 60% QE at low bias
    - 3x better than state of the art T2SLs

Measured spectral QE for three designs and bare detector material at 60K



Typical spectral QE at 60K w/o NA

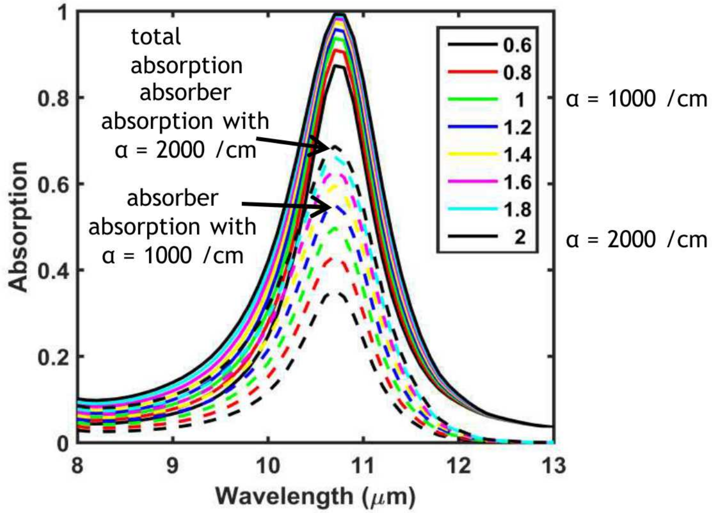


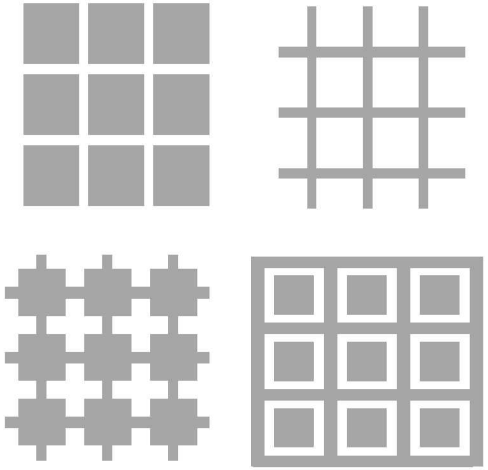


Nanoantennas allow us to have 3X the quantum efficiency.

Achieving Even Higher EQE

- Increase in absorption in the detector increases EQE
- Use modeling tools to maximize absorption in the absorber
  - Can use patch or mesh designs or a hybrid.
  - Designs may be capacitive or inductive.





We would like to optimize these structures using an accurate admittance model for nanoantenna elements.

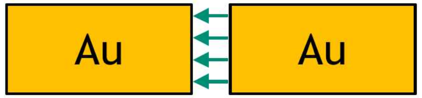
- very complicated expressions (but still analytic & fast to compute).
- provides design intuition - can guide numerical studies.
- can rapidly & accurately survey multidimensional parameter space.

Advanced Circuit Model

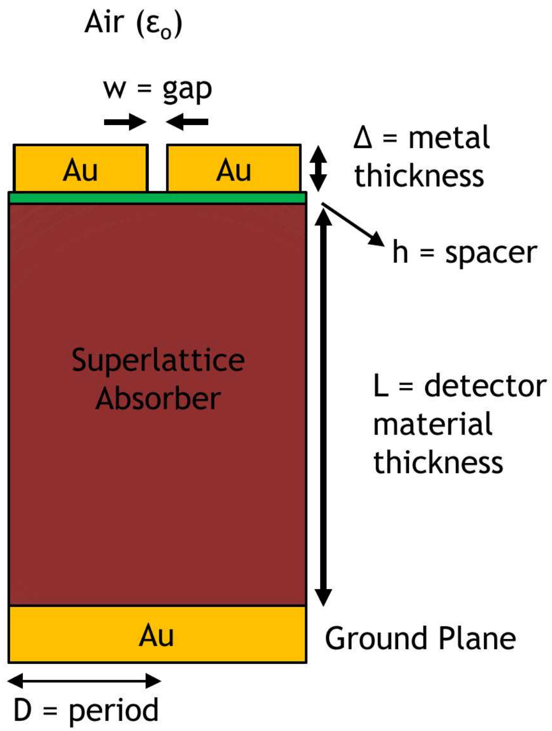
We have developed a very fast circuit model to let us design and optimize quickly while accurately modeling the structure.

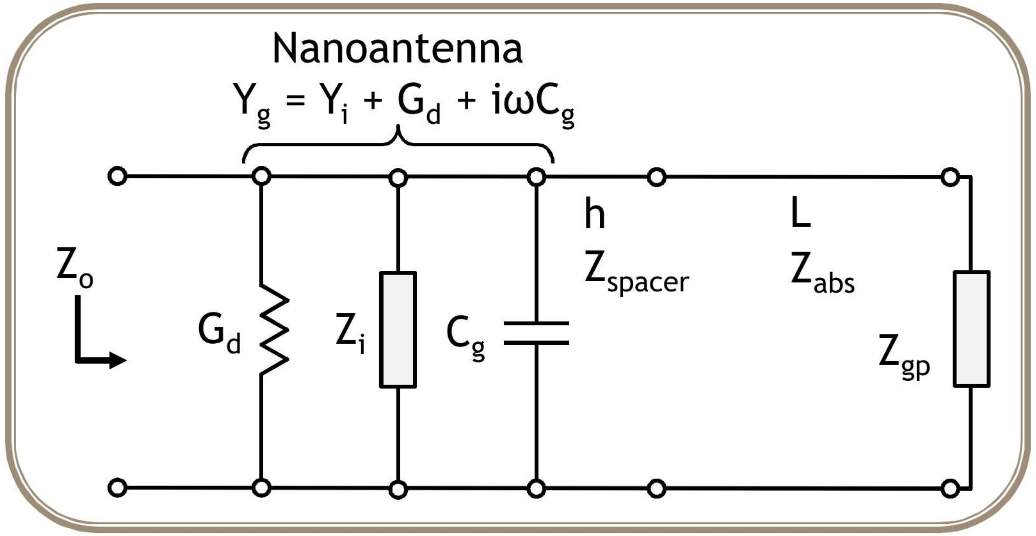
Based on the Tretyakov model. Features necessary to accurately model these structures:

- Finite metal conductivity in nanoantenna and ground plane.
- Finite metal patch thickness including field between metal elements



- Unequal permittivities above and below patch layer.

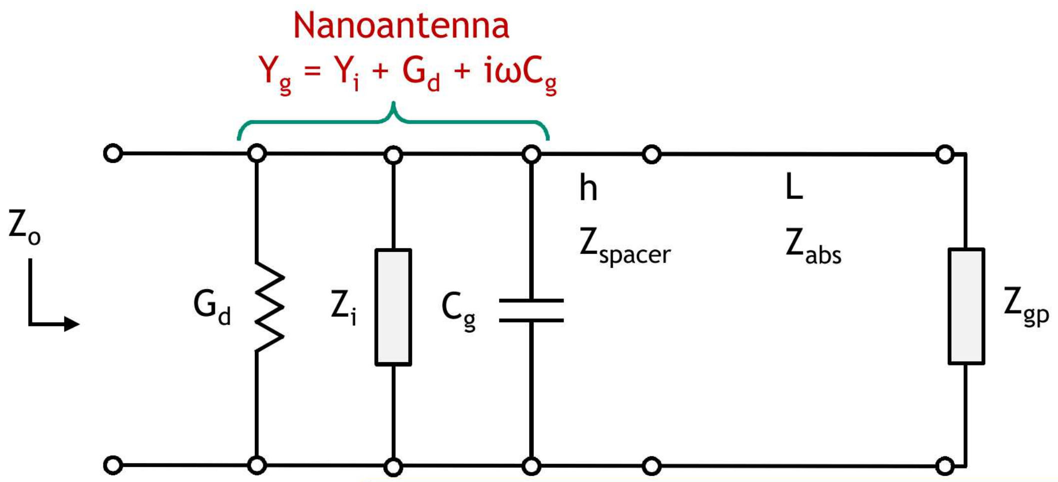


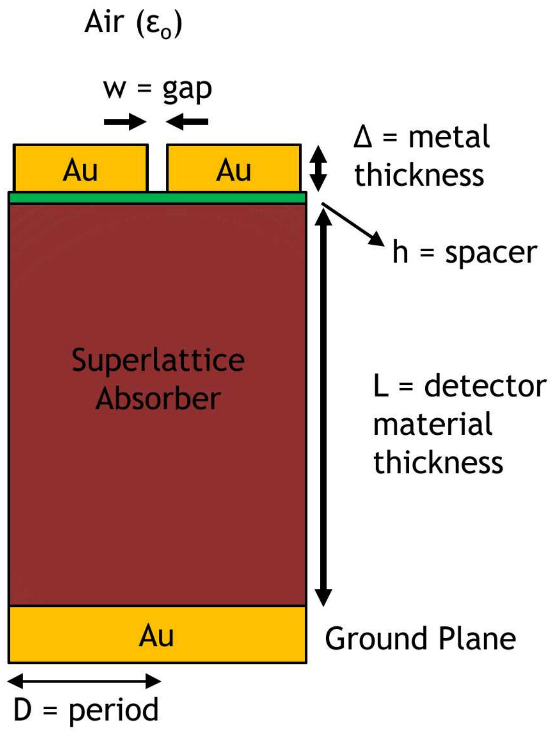


Advanced Circuit Model

Non-trivial to accurately account for the non-idealities described on previous slide.

Paper gives full details.





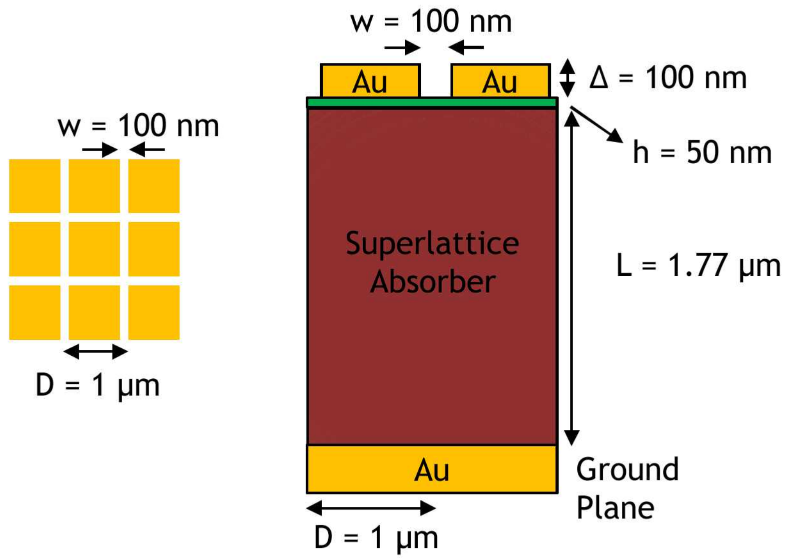
$$Y_g = Y_i + G_d - i\omega C_g \ , \ G_d - i\omega C_g = -i\omega(\varepsilon_0 + \varepsilon)\frac{1}{\pi} D \ln\left(\frac{D}{2\pi a_e}\right) \sim -i\omega(\varepsilon_0 + \varepsilon)\frac{1}{\pi} D \ln\left(\frac{2D}{\pi w}\right), \Delta / w << 1$$

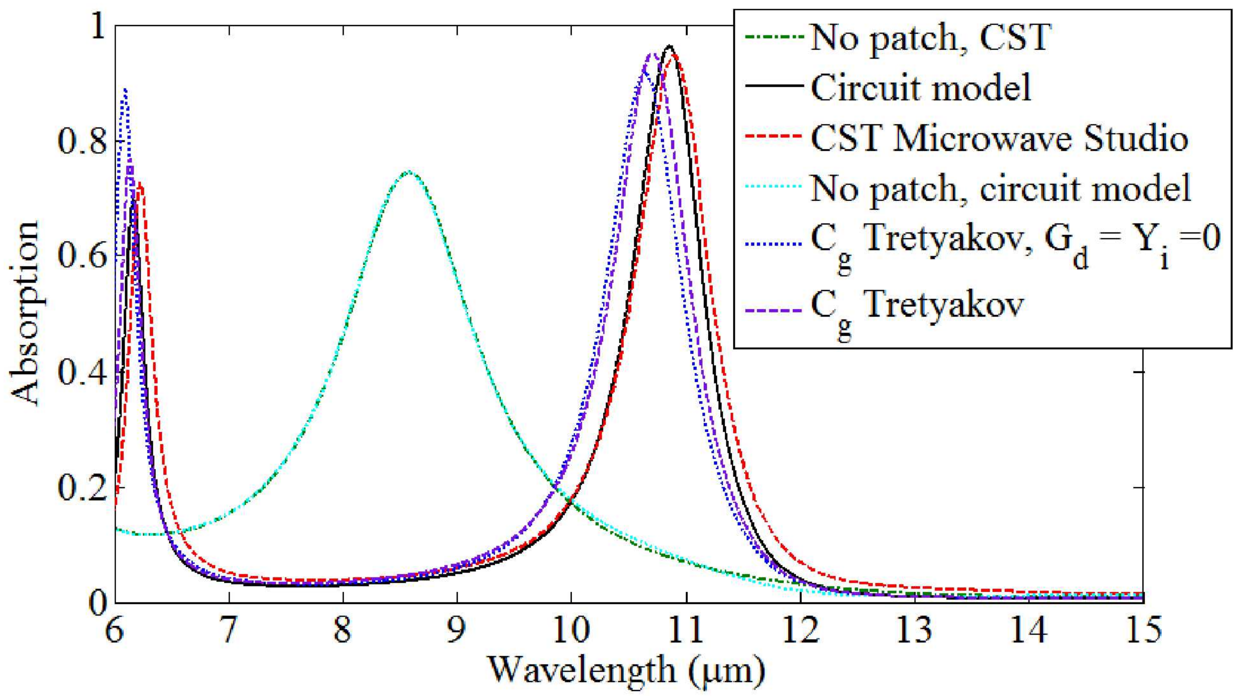
$$a_e: \left[\left(\varepsilon / \varepsilon_0 + 1\right)/2\right] \ln\left(a_e^0 / a^0\right) / \ln\left(a_e^{0\varepsilon} / a^0\right) \approx 1 + 0.67 \frac{\varepsilon / \varepsilon_0 - 1}{\varepsilon / \varepsilon_0 + 1.5} \frac{\Delta / w}{\Delta / w + 0.035}$$

S. Campione, L. K. Warne, M. D. Goldflam, D. W. Peters, and M. B. Sinclair, "Improved quantitative circuit model of realistic patch-based nanoantenna-enabled detectors," J. *Opt. Soc. of Amer. B*, vol. 35, pp. 2144-2152, Sept. 2018.

Comparison of Circuit Model to Electromagnetic Codes

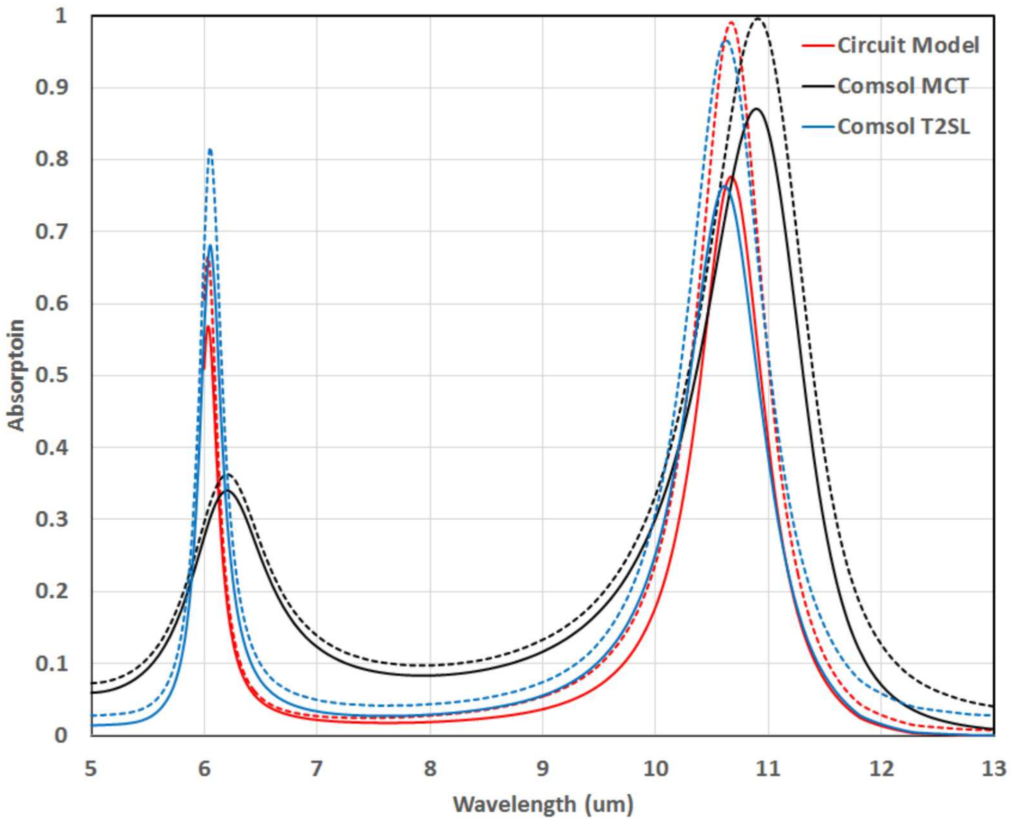
Comparison of circuit model with Tretyakov model and CST Microwave Studio





Excellent agreement between the circuit model and CST.

Use Circuit Model to Optimize Absorption



An example simulation showing that the concept also works for MCT detectors.

As MCT has a higher absorption coefficient than T2SLs we see an even higher EQE.

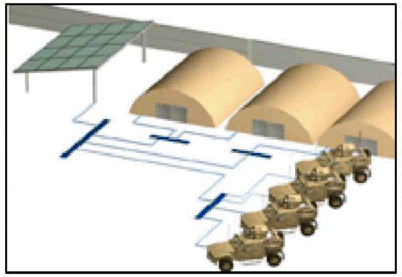
This architecture could make very high EQE, low-dark current MCT detectors.

Lowering the Temperature of Sodium Batteries for Grid Scale Storage

A Need for Grid-Scale Energy Storage

Renewable/Remote Energy

Grid Reliability

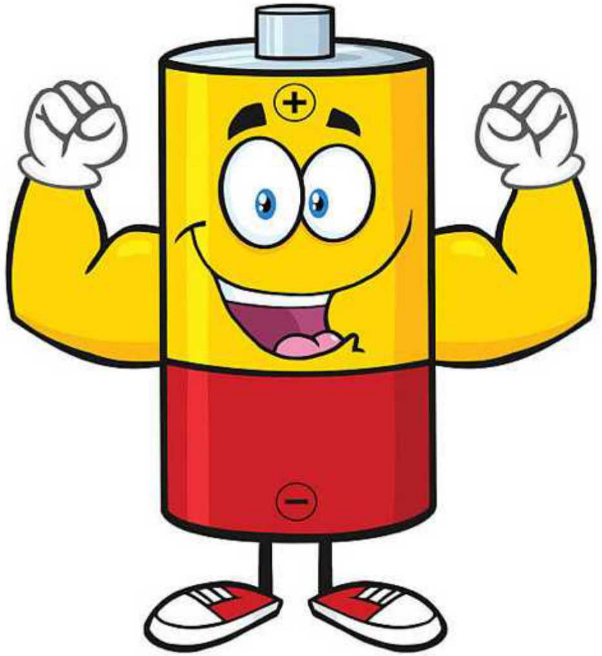


National Defense

Emergency Aid

As part of the DOE Office of Electricity efforts to create a modern, resilient, reliable, and agile grid system, we are developing new battery technology characterized by:

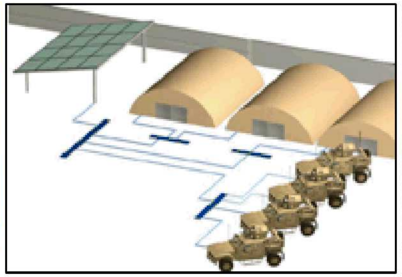
- Inherent Safety
- Long, Reliable Cycle Life
- Functional Energy Density (voltage, capacity)
- Low to Intermediate Temperature Operation
- Low Cost and Scalability



Sodium Batteries

Renewable/Remote Energy

Grid Reliability



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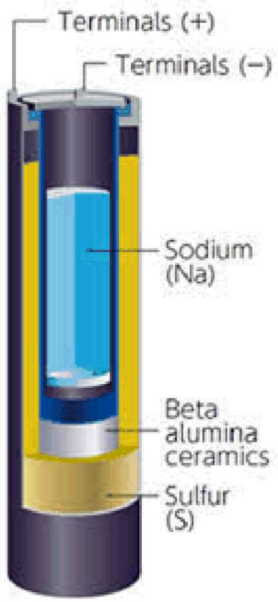
Sodium-based batteries

- 6th most abundant element on earth.
- 5X the annual production of aluminum.
- Proven technology base with NGK Sodium/Sulfur (NaS) and FzSoNick ZEBRA (Na-$NiCl_2$) systems.
- Utilize zero-crossover solid state separators.
- Favorable battery voltages (>2V).



Na-S (E_{cell} ~ 2V)

$2Na + 4S \leftrightarrow Na_2S_4$

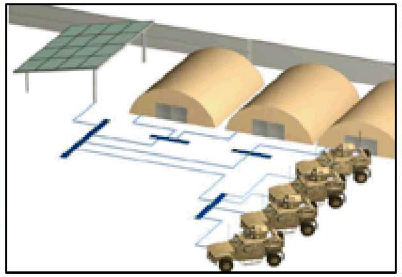
Na-$NiCl_2$ (E_{cell} ~ 2.6V)

$2Na + NiCl_2 \leftrightarrow 2Na^+ + 2Cl^- + Ni(s)$

Sodium Batteries


Renewable/Remote Energy

Grid Reliability



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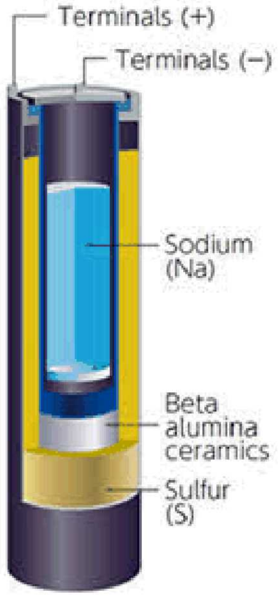


Na-... V)

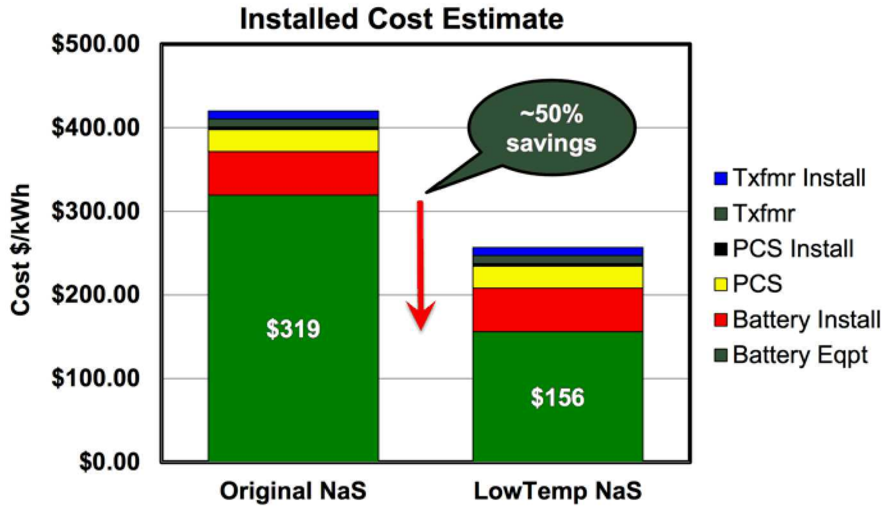
2Na ... $Na^+ + 2Cl^- + Ni(s)$

~300°C Operation!

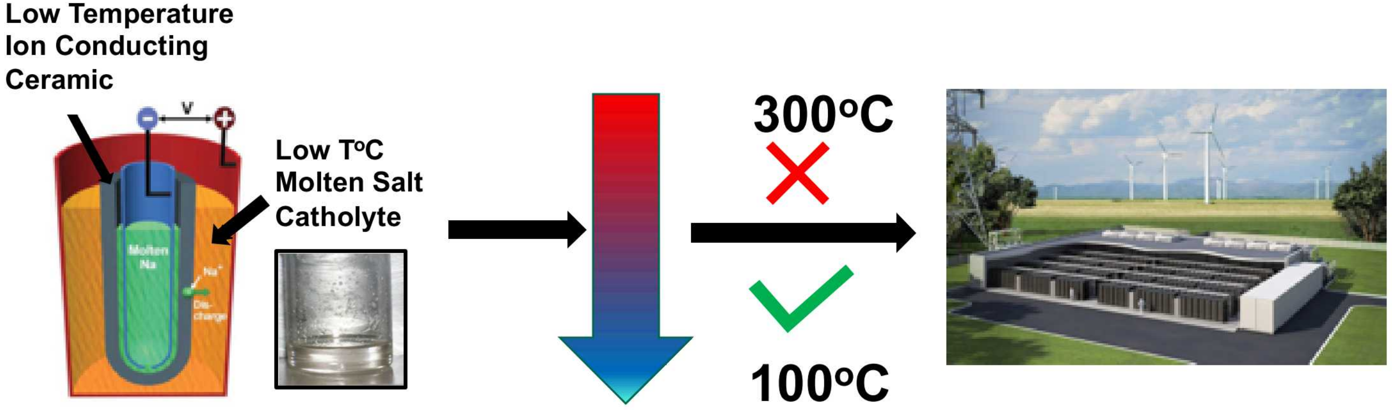
Lowering Battery Operating Temperature to Drive Down Cost

Our Objective: A safe, reliable, molten Na-based battery that operates at drastically reduced temperatures (near 100°C).

- Improved Lifetime
  - Reduced material degradation
  - Decreased reagent volatility
  - Fewer side reactions
- Lower material cost and processing
  - Seals
  - Separators
  - Cell body
  - Polymer components?
- Reduced operating costs
- Simplified heat management costs
  - Operation
  - Freeze-Thaw



Gao Liu, et al. "A Storage Revolution." 12-Feb-2015 (online): https://ei.haas.berkeley.edu/education/c2m/docs/Sulfur%20and%20Sodium%20Metal%20Battery.pdf

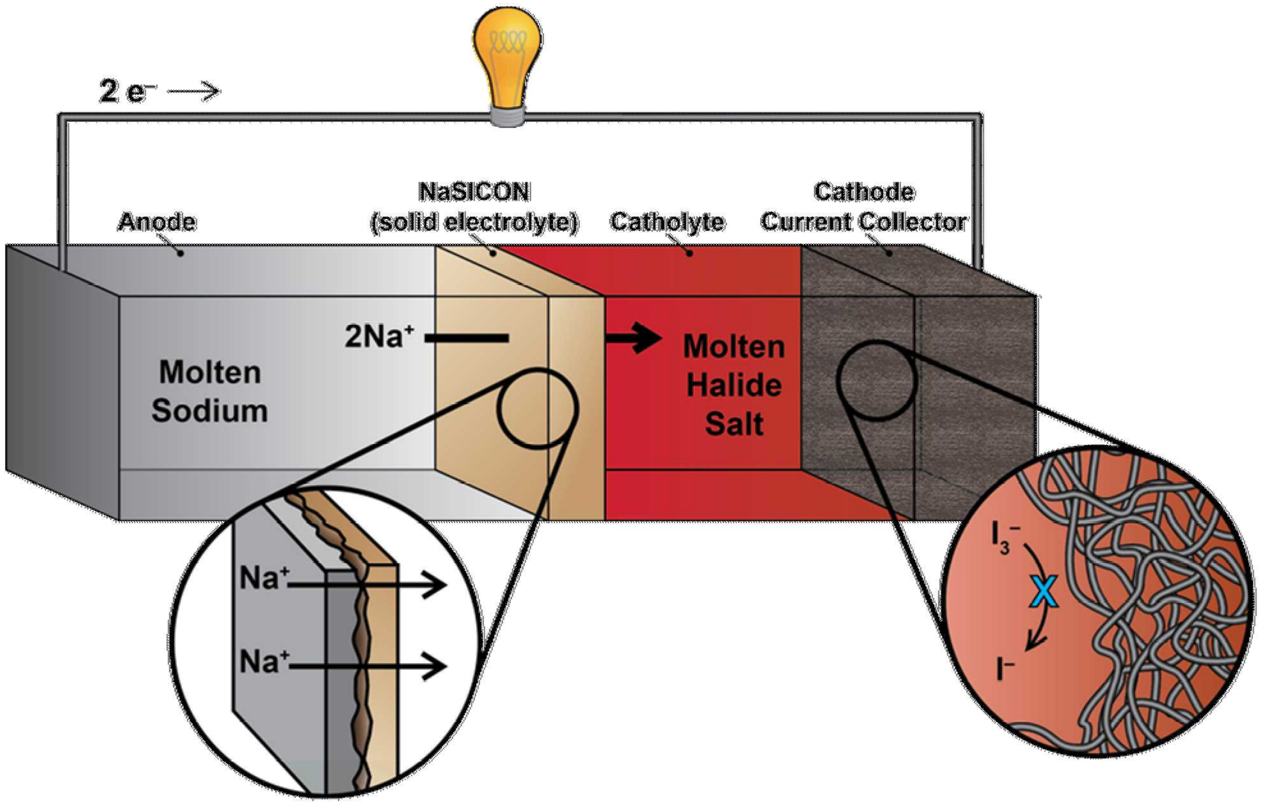


Low Temperature Molten Sodium (Na-NaI) Batteries

Realizing a new, low temperature molten Na battery requires new battery materials and chemistries.

Ingredients for Success

- Molten Na anode
- Highly Na^+-conductive, zero-crossover separator (e.g., NaSICON)
- 25 mol% NaI in AlX_3 catholyte
- *No complications from solid state electrodes!*



Na-NaI battery:

$Na \rightarrow Na^+ + e^-$ $E^0 = 0V$

$I_3^- + 2e^- \rightarrow 3I^-$ $E^0 = 3.24$

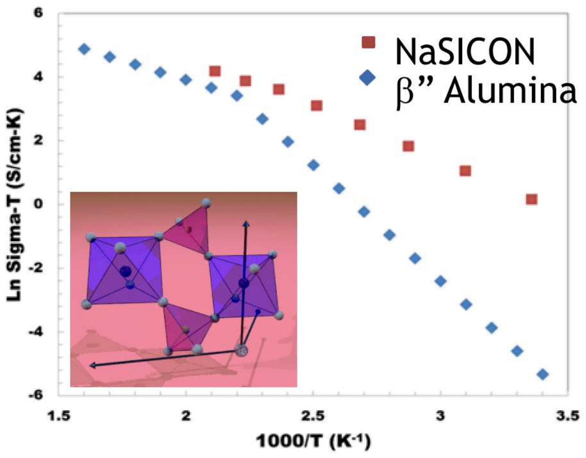
$2Na + I_3^- \rightarrow 2Na^+ + 3I^-$ $E^0_{cell} = 3.24V$

Martha Gross

NaSICON Separator

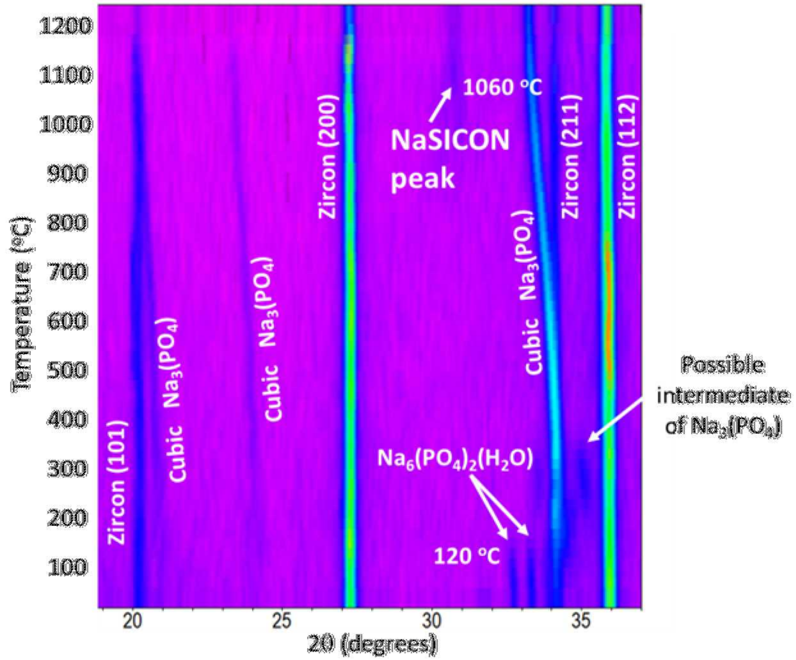
Key Qualities of NaSICON Ceramic Ion Conductors

- $Na_3Zr_2PSi_2O_{12}$
- High Na-ion conductivity (>10^{-3} S/cm at 25°C)
- Chemical Compatibility with Molten Na and Halide salts
- Zero-crossover



NaSICON calcined to remove hydrates, sintered at 1230°C, yields >94% density and >0.4 mS/cm at 25°C.

These ceramics are suitable for lab-scale testing of molten sodium batteries.



- VTXRD shows conversion of Zircon and cubic $Na_3(PO_4)$ to NaSICON starting near 1100°C
- Hydrate form of $Na_3(PO_4)$ up to 120°C, converts to cubic $Na_3(PO_4)$ at ~300°C.

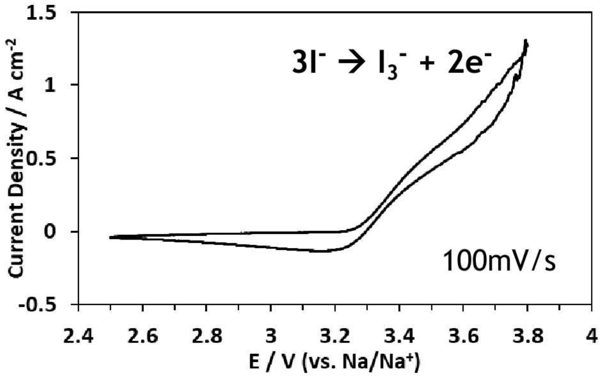
Early Low Temperature Na-Battery Performance

Deliberate materials approach reveals low temperature NaI-based molten salts.

The NaI-$AlBr_3$ catholyte system is molten and exhibits excellent electrochemical behavior at reduced operating temperatures.

- 25:75 NaI-$AlBr_3$salt completely molten at 90 °C
- Large fully molten capacity range (~5-25 mol% NaI)

Iodide is electrochemically active in 25 mol% NaI-$AlBr_3$ at 90°C



Stephen Percival

Early Low Temperature Na-Battery Performance

First demonstration of molten Na-NaI battery at 100-110°C.

The NaI-$AlBr_3$ catholyte system is molten and exhibits excellent electrochemical behavior at reduced operating temperatures.

- 25:75 NaI-$AlBr_3$salt completely molten at 90 °C
- Large fully molten capacity range (~5-25 mol% NaI)

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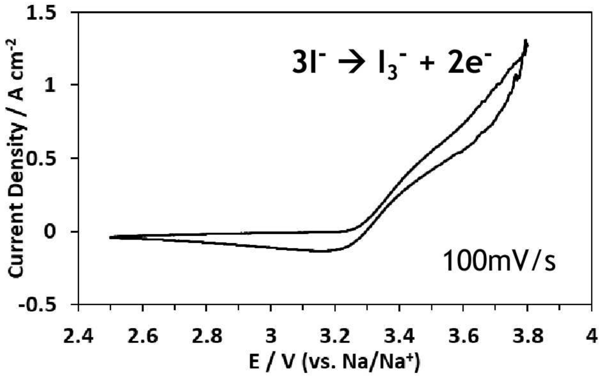
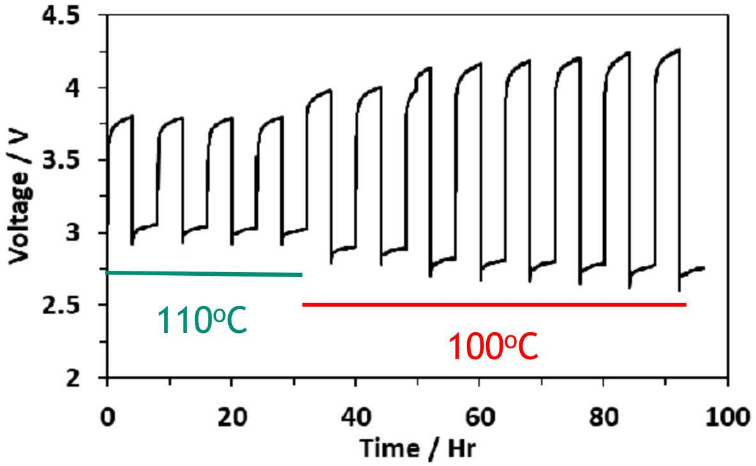
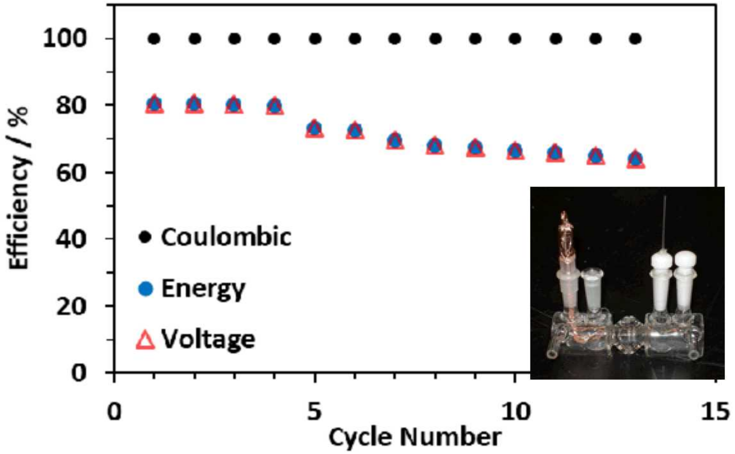




Battery cycling at **100-110°C**!



25 mol% NaI-$AlBr_3$ with NaSICON separator.

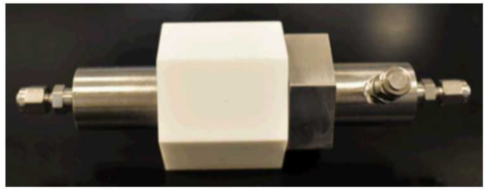
Stephen Percival

Identifying a Viable Na-Battery Test Platform

Cell geometry, interfacial interactions, and materials compatibility were identified as key design elements.

Re-Engineered Cell Variants

A functional cell design is critical to prototype development and testing.

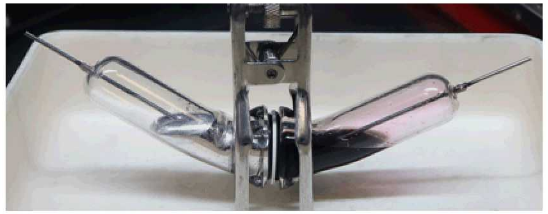


Many new cell designs and geometries built and tested (7 different types!)

Some designs were time consuming, laborious and could be **<u>used only once!</u>**

New Cell Designs

Enable easy assembly, high throughput and functional geometry



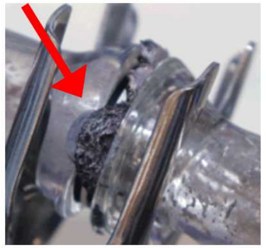
Includes 3 designs that are fully interchangeable and reusable

Importance of Seals

Testing failures in many prototypes was due to compromised seals.

<u>Sodium Compatible Seal Material</u>

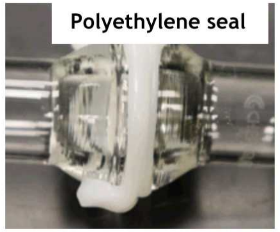
Sodium reacting with the Kalrez o-ring



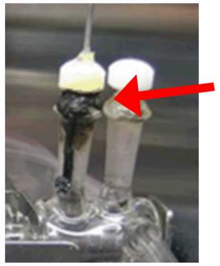
Polyethylene seals from molten polyethylene to seal the sodium side

Not re-useable and hard to apply properly

Identified new EPDM o-rings that do not react with molten Na

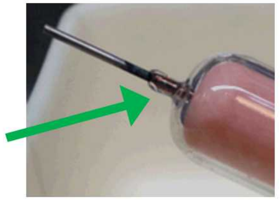


<u>Molten Salt Compatible Seal Material</u>



Vapors from molten salt aggressively attacking the epoxy seals

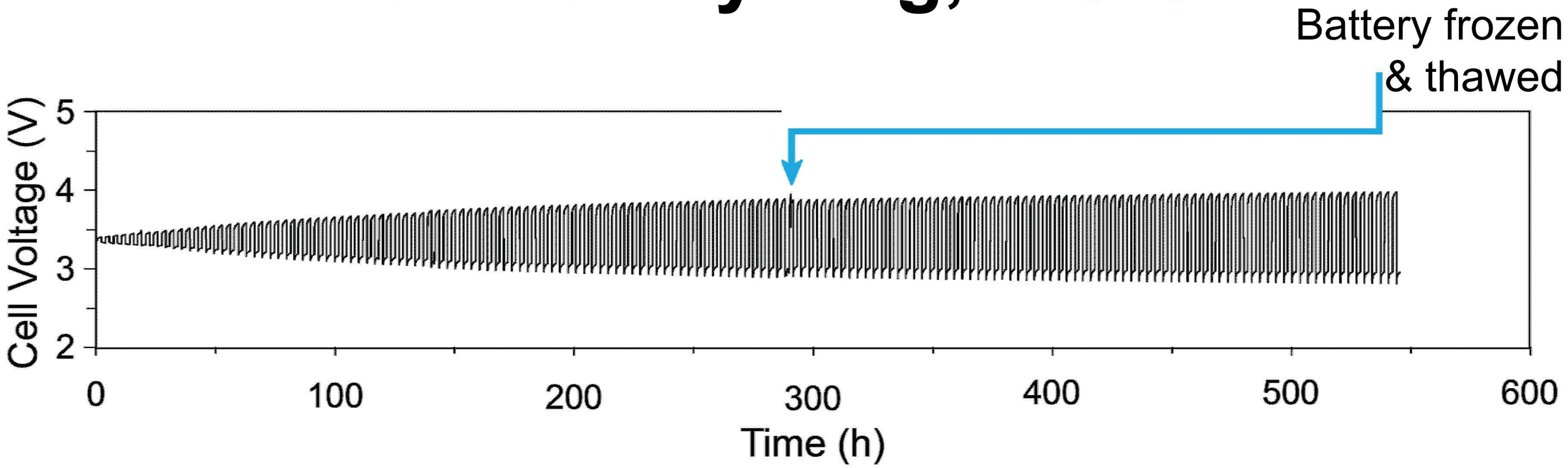
Glass to metal seals eliminate unwanted side reactions from salt vapors



Stephen Percival

This Year's "Really Cool" Hurrah!

Full Cell Cycling, 110°C

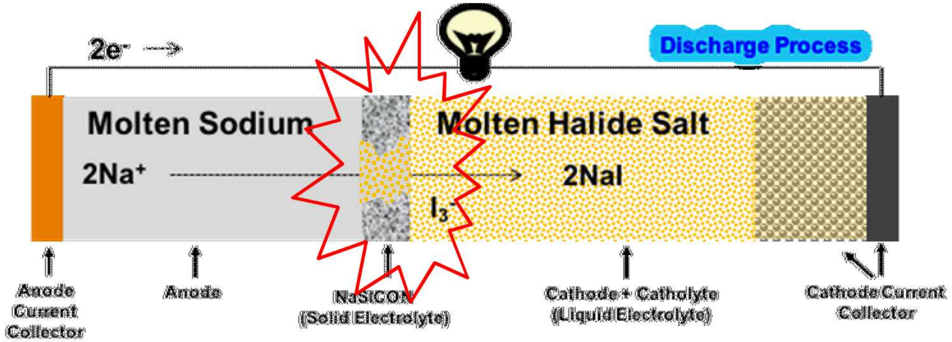


- Integration of Sn-based coating and activated CF enables long-term battery cycling: **Battery achieved 200 cycles!**
- Even after freeze/thaw, interfaces remain intact with uninterrupted cycling!

Martha Gross

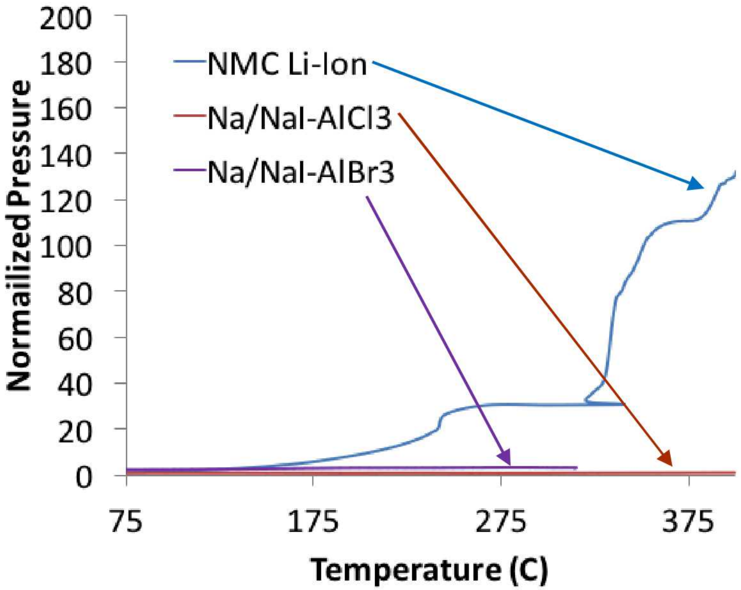
Evaluating Potential Hazards of "Failed" Na-NaI Batteries

- Inherent Safety
- Long, Reliable Cycle Life
- Functional Energy Density (voltage, capacity)
- Low to Intermediate Temperature Operation
- Low Cost and Scalable



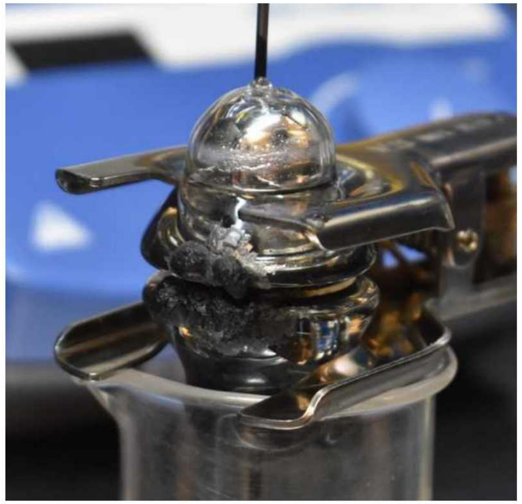
Simulating separator failure, metallic Na and NaI/AlX_3 were combined and heated.

Byproducts of reaction are aluminum metal and harmless sodium halide salts.



Accelerating rate calorimetry reveals that Na-NaI/AlX_3 mixtures exhibit:

1) *no significant exothermic behavior*
2) *no significant gas generation of pressurization*



Failed separator led to termination of battery, but no significant hazardous conditions.

Summary

Project Objective: A safe, reliable, molten Na-based battery that operates at drastically reduced temperatures (near 100^{o}C).

Identified a low temperature, functional NaI-based molten catholyte and demonstrating initial battery cycling at 100^{o}C, in FY19, we…

- ✓ Redesigned Na battery testing platform, accounting for cell materials compatibility, sealing, and interfacial chemistry.
- ✓ Produced functional NaSICON for use in low temperature prototype test cells.
- ✓ Discovered several approaches to improve critical Na-wetting of NaSICON at 100^{o}C.
  - ✓ Polishing
  - ✓ Na-bake (carmelized NaSICON)
  - ✓ Sn-based coating
- ✓ Revealed that activating interfaces on "high" surface area carbon felt leads to significant reduction of cell overpotentials.
- ✓ Comprehensive integration of new cell design with new cell materials, demonstrated first ever long-term cycling (200 cycles!) of molten Na-NaI battery at 110^{o}C.

Graphene Oxide Membranes for improved Water Desalination

Graphene Oxide/Polymer Desalination Membranes

Motivation

- Robust, chlorine tolerant desalination membranes are need for water recycling and grey water reuse
- Thermoelectric water recycling requires membranes with high rejection for divalent ion loads
- Contaminants of emerging concern must be removed for grey water reuse

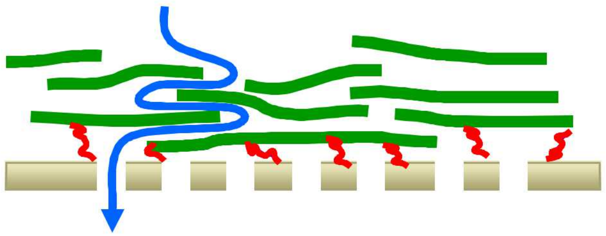
Industry benchmarks for reverse osmosis membranes

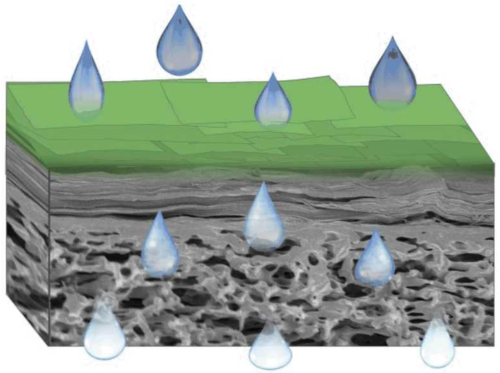
- Permeance ~ 3 LMH/bar
- Rejection > 98%
- Intolerant to chlorine > 0.1 mg/L

$$\frac{L}{m^2 * hr * bar} = LMH/bar$$

The GO/polymer membranes comprise three key layers

Laminar graphene oxide, covalent linker molecules and porous polymer support provide ion rejection, membrane integrity, and mechanical durability.



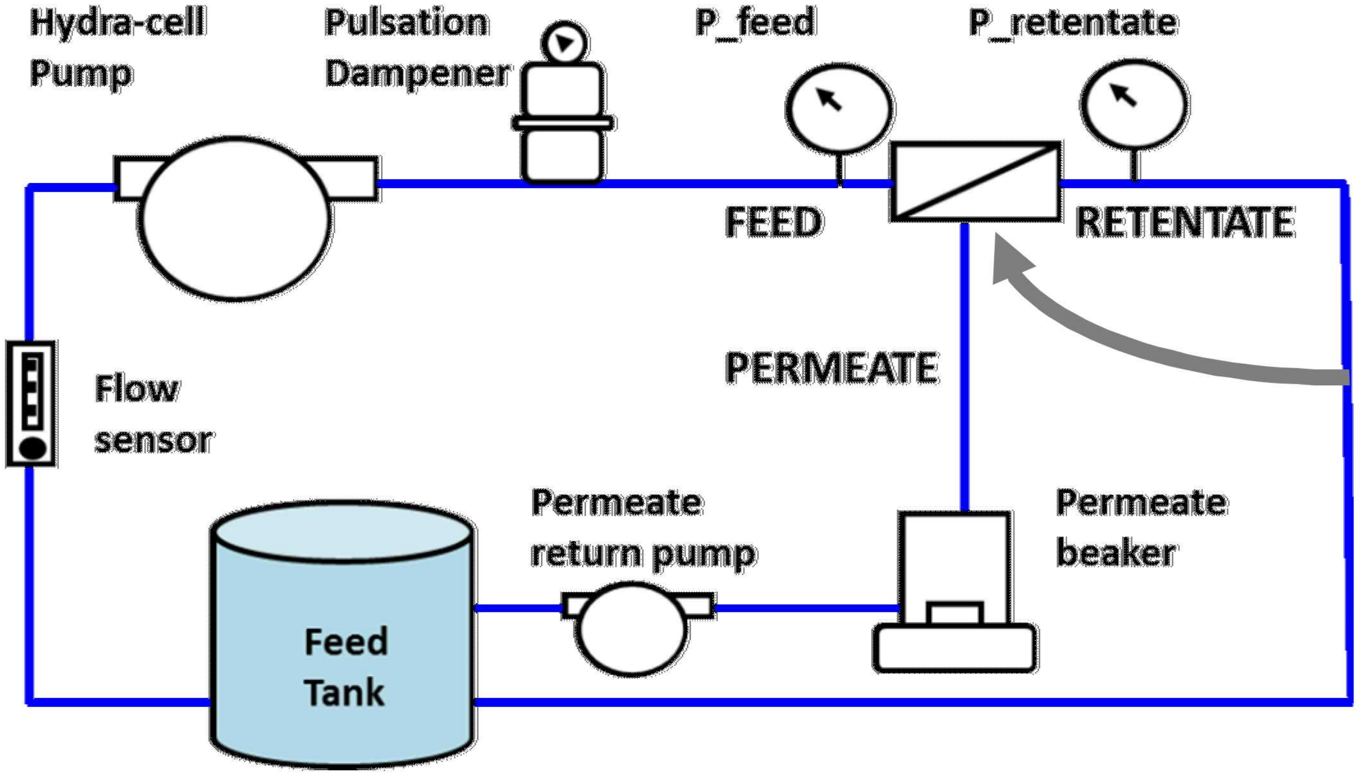


~2" x 4" membrane

What is the optimum porous polymer support?

How do we optimize the laminar GO structure for maximum flow, rejection, and durability?

Automated cross-flow system allows for month-long desalination tests



~2” x 4” membrane

Control

Feed tank water salinity

Driving pressure

Monitor

Conductivity, feed & permeate

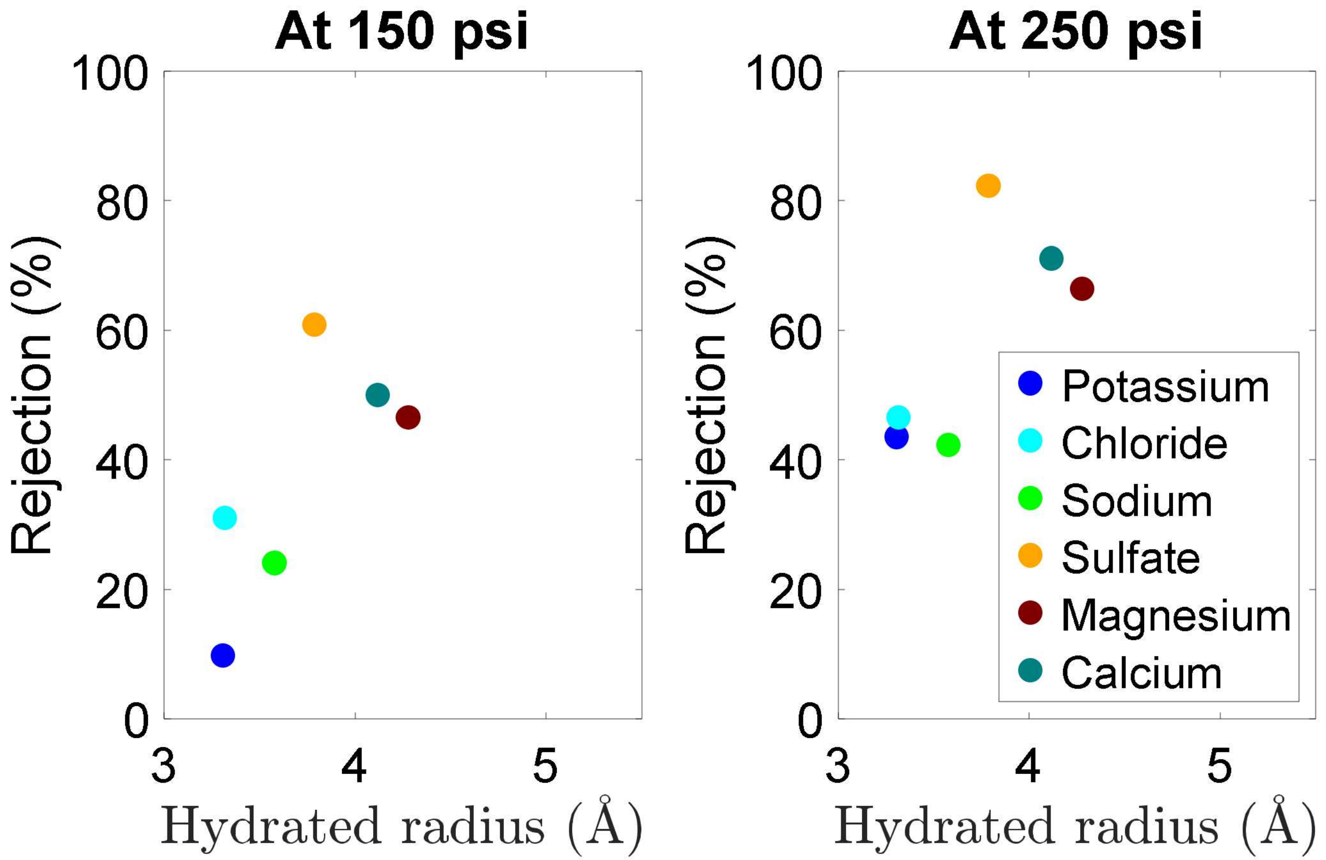
Permeate flow

Calculate

Rejection (%)

Permeance (LMH/bar)

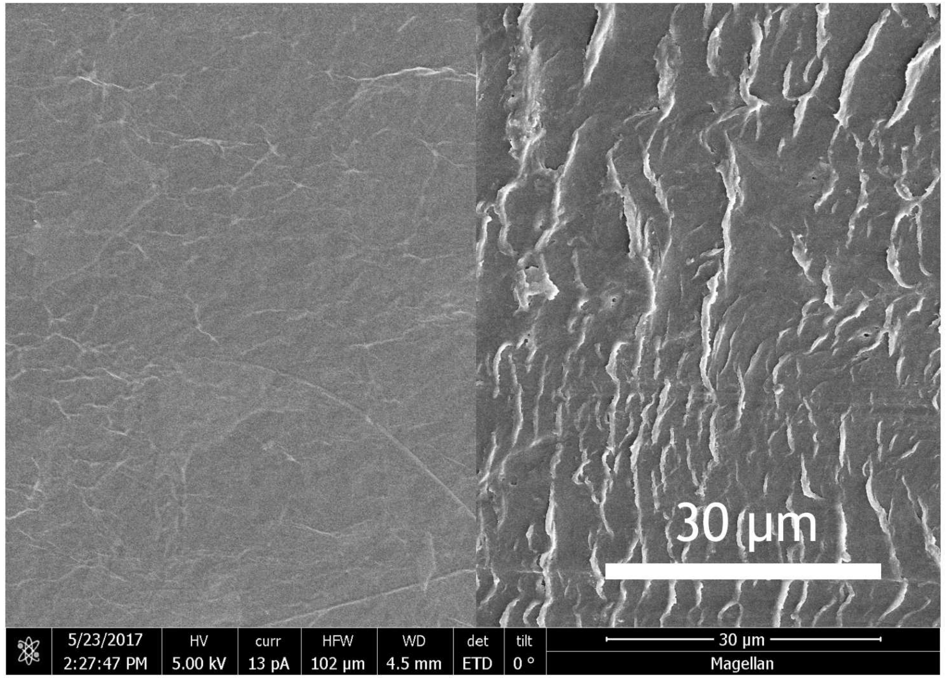
Ion rejection increases with increasing hydrated ion radius and driving pressure



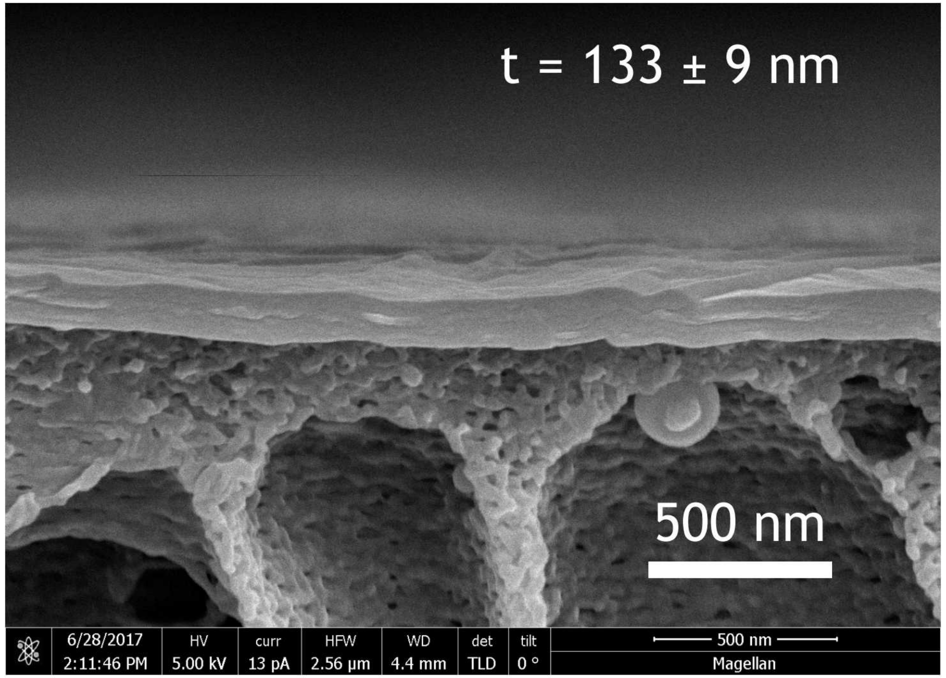
Constant permeance of 0.3 LMH/bar

- Membrane displayed outstanding tolerance at 0.5 mg/L chlorine
- Good overall rejection performance on West Phoenix power plant cooling tower water

Graphene Oxide on Ultrafiltration Support

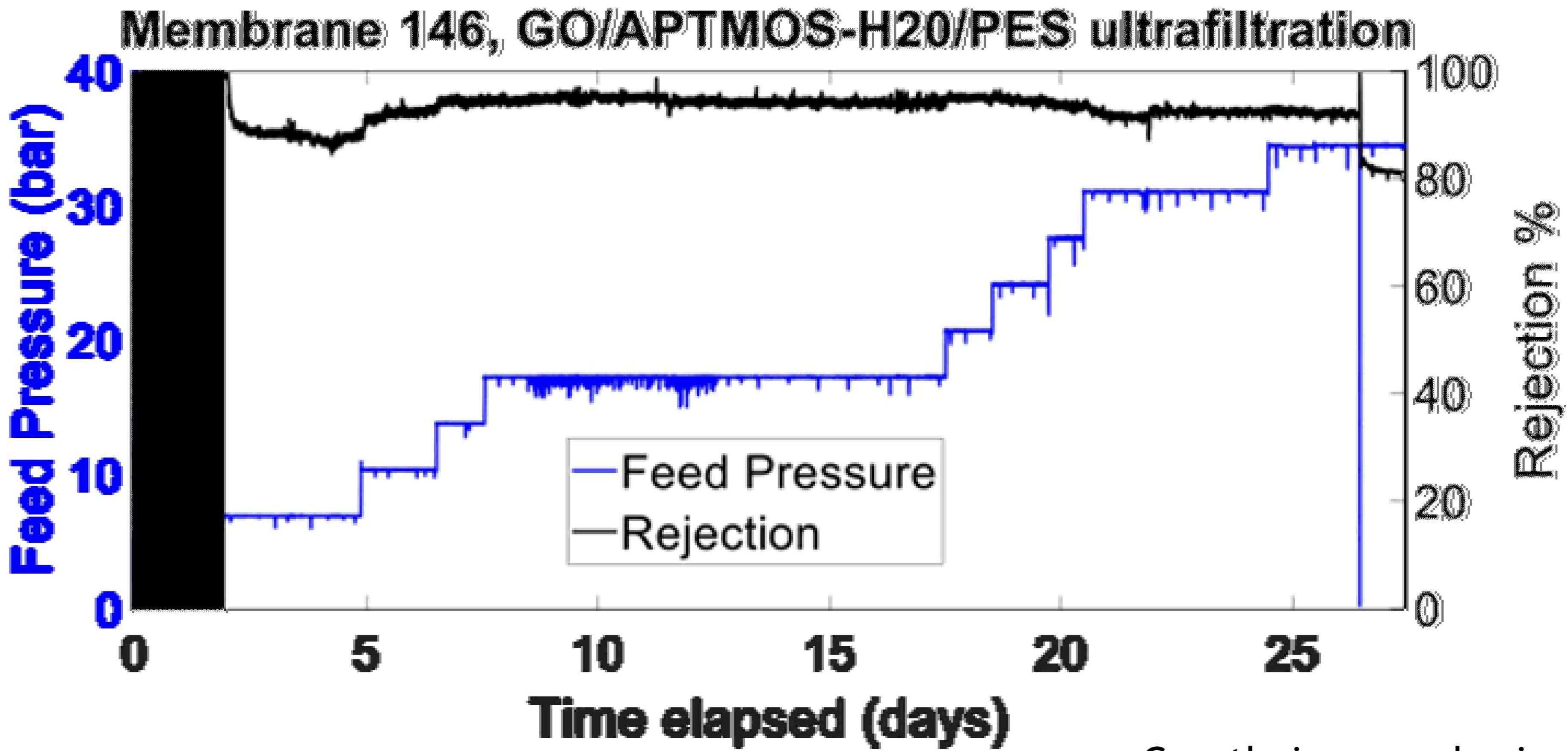


- Assembled GO composite (left) using ultrafiltration membrane (right)



- GO/APTMOS/PES, water functionalized, ultrafiltration substrate, 200 kDa cutoff

Graphene Oxide on Ultrafiltration Support



- Greatly improved rejection with sulfate rejection over 95% (net conductivity difference shown)
- Permeances of 0.1-1 LMH/bar with ultrafiltration supports
- Mem146: 0.4 LMH/bar DI permeance

Graphene Oxide on Ultrafiltration Support

Mem146	Feed conc. (ppm)	Permeate conc. (ppm)	Rejection at 100 psi (%)	Feed conc. (ppm)	Permeate conc. (ppm)	Rejection at 300 psi (%)
DMMP	96	7.0	**92.7%**	102.4	5.5	**94.6%**
Ibuprofen	10.6	93 ppb	**99.1%**	10.4	111 ppb	**98.9%**
Chlorate	68.5	18.5	**72.9%**	70.6	9.7	**86.2%**
Nitrate	50.0	3.3	**93.5%**	49.1	nd	**100%**
Phosphate	76.3	3.9	**94.8%**	71.2	2.2	**96.9%**
Sulfate	352.9	6.6	**98.1%**	365.1	4.9	**98.7%**

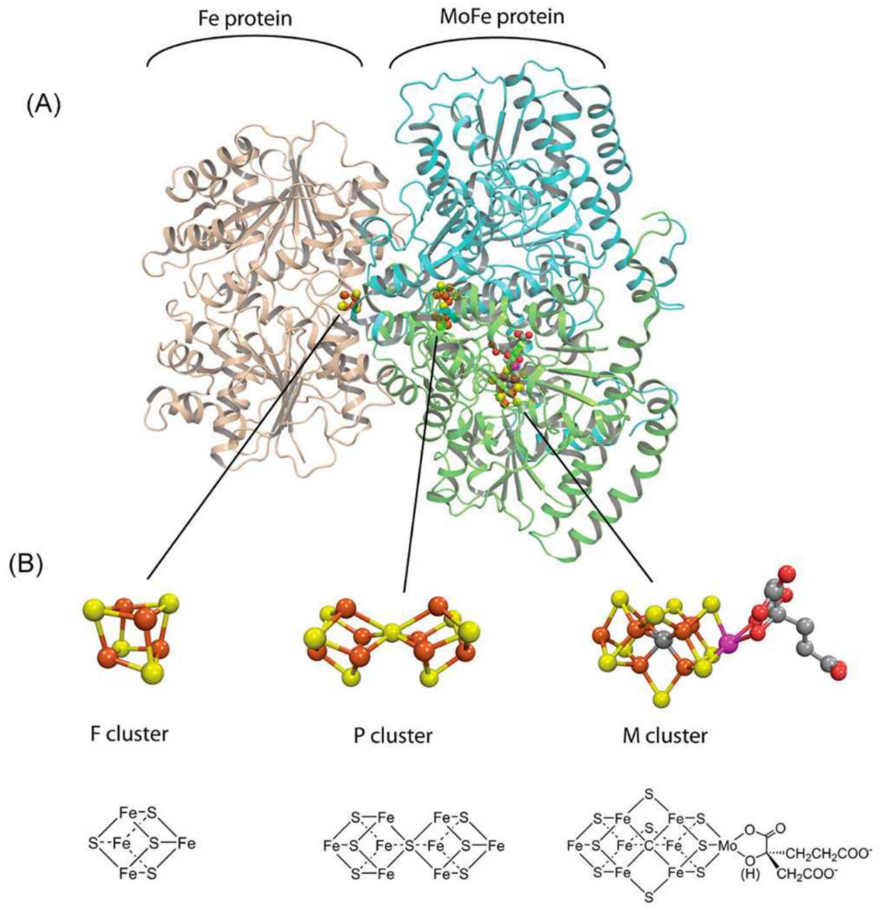
- Membranes have been exposed up to 3 mg/L free chlorine with no adverse effects
- Achieved consistent, pressure-tunable ion rejection with divalent ion rejections > 95% as well as significant rejection of contaminants of emerging concern

Improved Catalyst for Ammonia Production to Reduce the Cost of Food Production

Nitrogen Reduction Catalysis

- Iron catalyzed Haber – Bosch process has been the standard method for nitrogen reduction since the early 20th century
- Produces Ammonia at temperatures above 350C and pressures over 150 atm
- As a reliable source of nitrogen for fertilizer it is key to feeding the growing population
- Estimates indicate the Haber – Bosch process is responsible for over 1% of the world's energy consumption
- How can we reduce the temperature of this process and lower energy consumption?

Nitrogenase: Electron Source, Shuttle and N_2 binding



Hoffman et al, Mechanism of Nitrogen Fixation by Nitrogenase: The Next Stage. DOI 10.1021/cr400641x

Biological inspiration for catalyst design

Nitrogenase reaction:

$$N_2 + 8H^+ + 8e^- \rightarrow 2NH_3 + H_2$$

The F cluster (Fe protein) is the electron donor to the M cluster

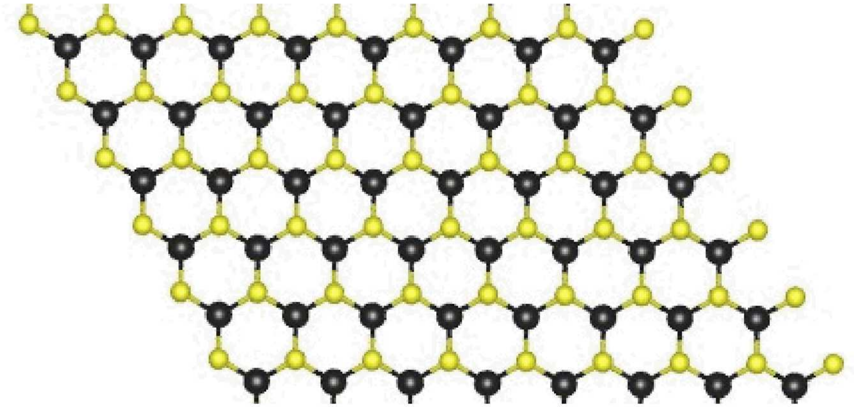
MoFe protein:

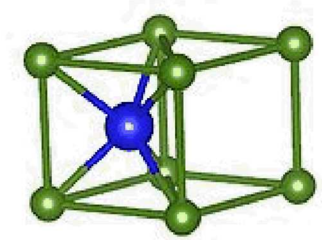
- P-cluster: electron shuttle
- **M cluster**: active site

Some debate on actual binding site in M cluster.

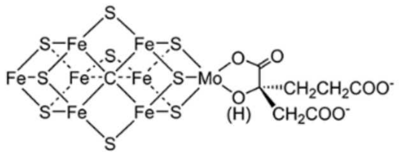
3 or 4 electrons accumulate in M cluster before N2 binds

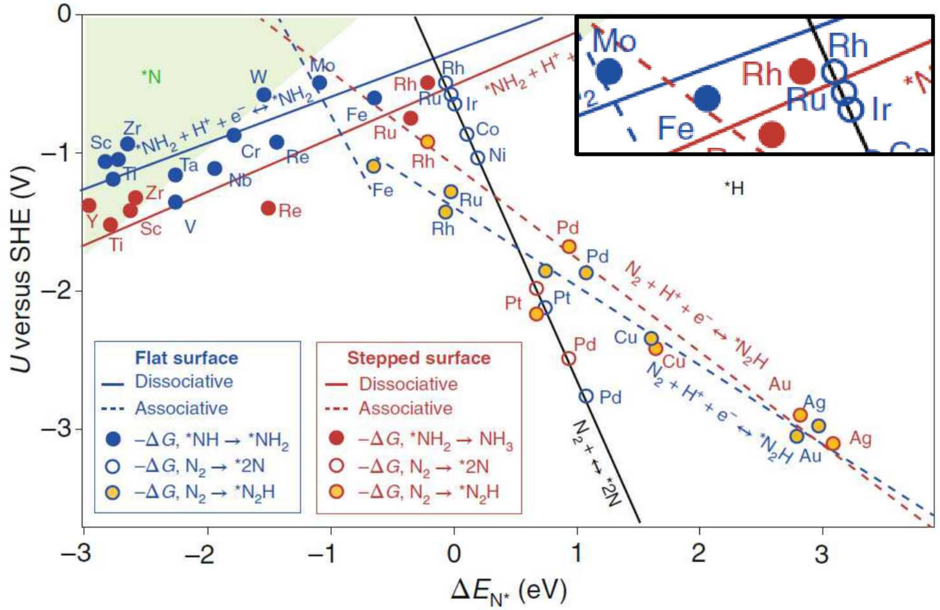
M cluster mimic?





M cluster



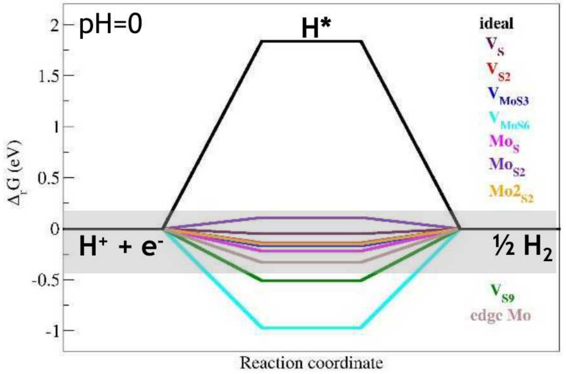


Suryanto, B.H.R. *et al.* Nature Catalysis 2 (2019) 290-296

- Trigonal prismatic 2H MoS2 resemblance to M cluster protein
- MoS2 can incorporate elements from Sabatier plot of NRR active metals (Mo, Fe, Rh)

DFT Identification of Potential **NRR** Sites in MoS_2

DFT calculated free energy diagrams for HER on 2H MoS_2
ideal plain, edge, and different plain defects
single-, few-atom vacancies, antisites from Ouyang et al. *Chem. Mater.* 28, 4390 (2016);
optB86b-vdW level



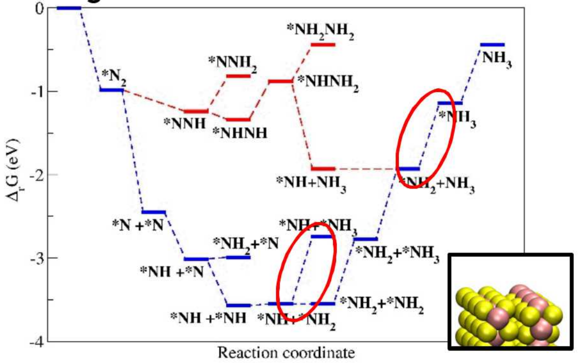
-0.2 < $\Delta_r G_{H^*}$ < 0.2eV - good HER activity but low N2RR efficiency

Conclusions

- out of 20 active site of MoS_2 tested (7 grain boundaries, 10 single-/few- atom vacancies, antisites, 2 edge sites, and ideal plain) edge Mo sites are the most promising sites for N2RR, cell potentials of at least -0.8 V needed to drive N2RR to ammonia.
- Recommendation: to increase the activity of the basal plain DFT suggests to substitute S or Mo with elements other than Mo – test other 2D materials of interest

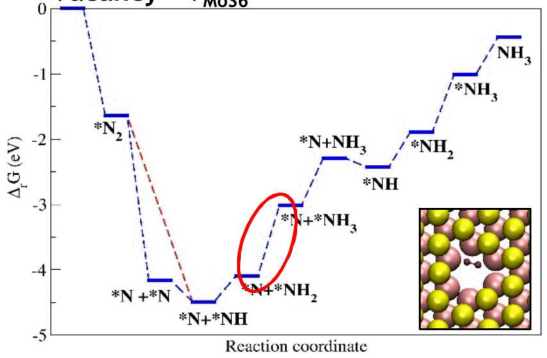
DFT calculated free energy diagrams for N2RR on most promising sites of 2H MoS_2 (exothermic N_2 adsorption); optB86b-vdW level (vdW-corrected functional)

Edge Mo



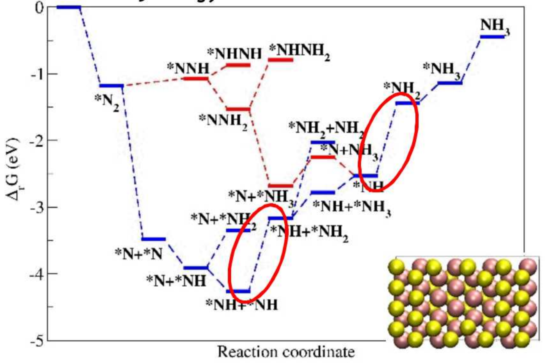
- N2RR *via* dissociative mechanism
- Low barrier for N_2 dissociation 0.56 eV
- N2RR onset potential -0.80 V

Vacancy - V_{MoS6}



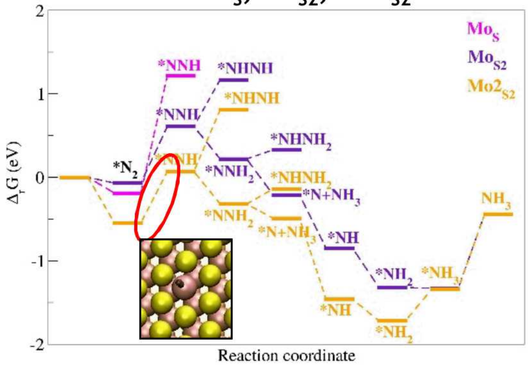
- N2RR *via* dissociative mechanism
- N2RR onset potential as high as -1.1 V

Vacancy – V_{S9}



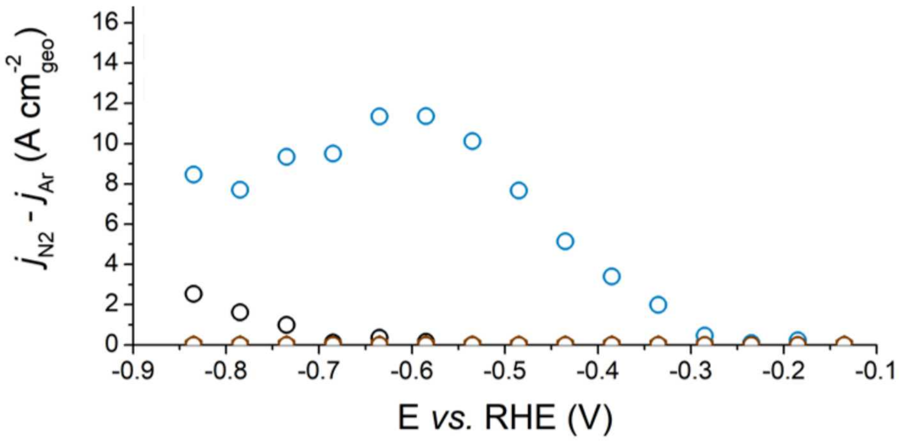
- N2RR *via* dissociative mechanism
- N2RR onset potential -1.09 V

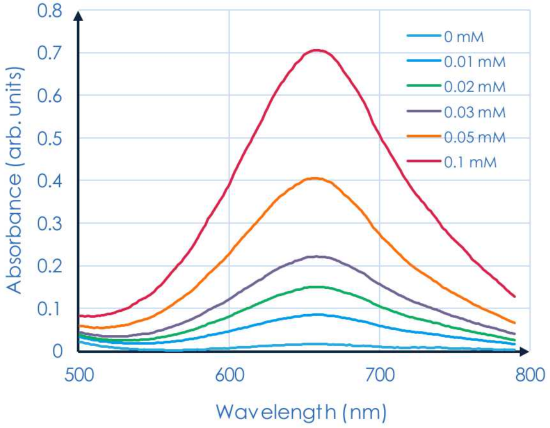
Antisites - Mo_S, Mo_{S2}, $Mo2_{S2}$

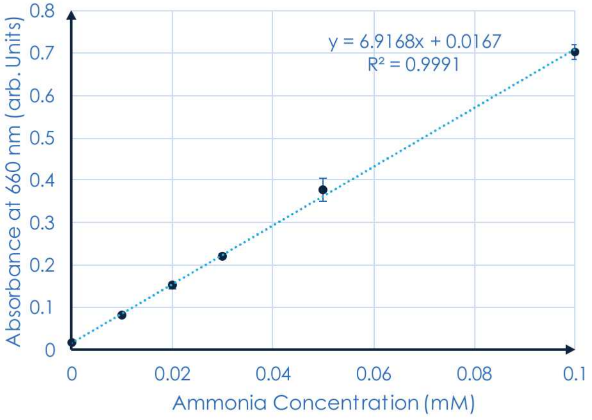


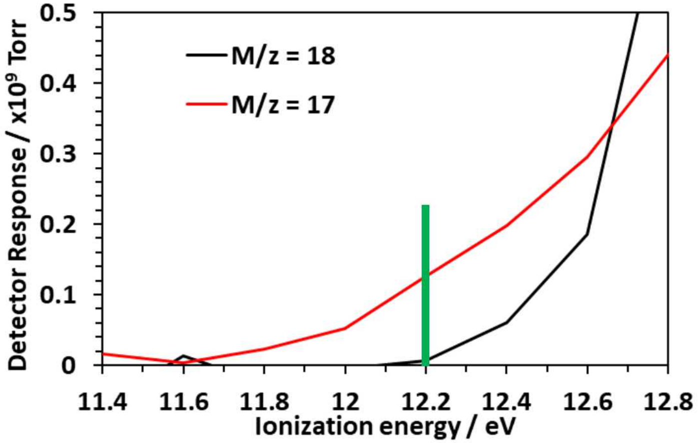
- N2RR onset potential on Mo_S at least -1.41 V
- N2RR onset of -0.68 V on Mo_{S2} and -0.62 V $Mo2_{S2}$

Catalyst testing









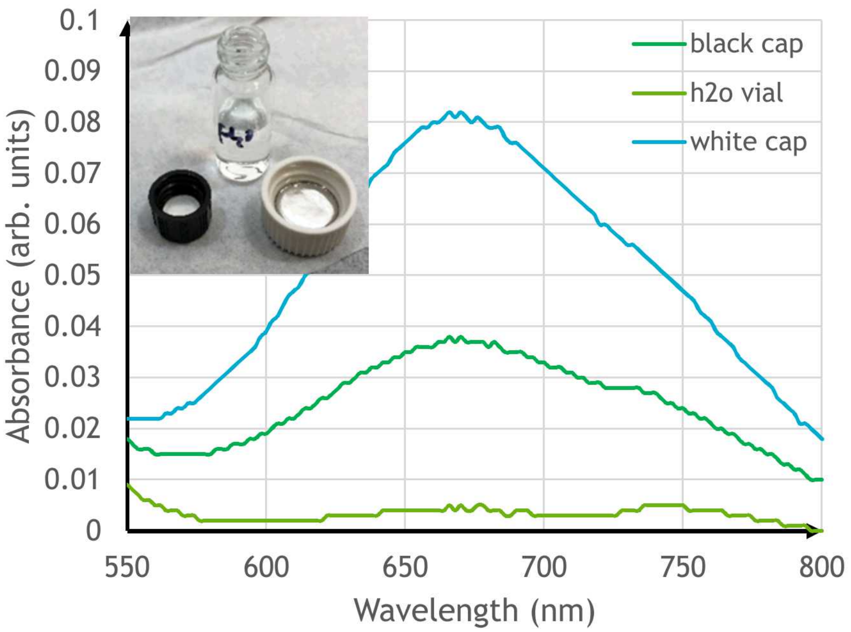
Current measurement with N2 and Ar feed gas

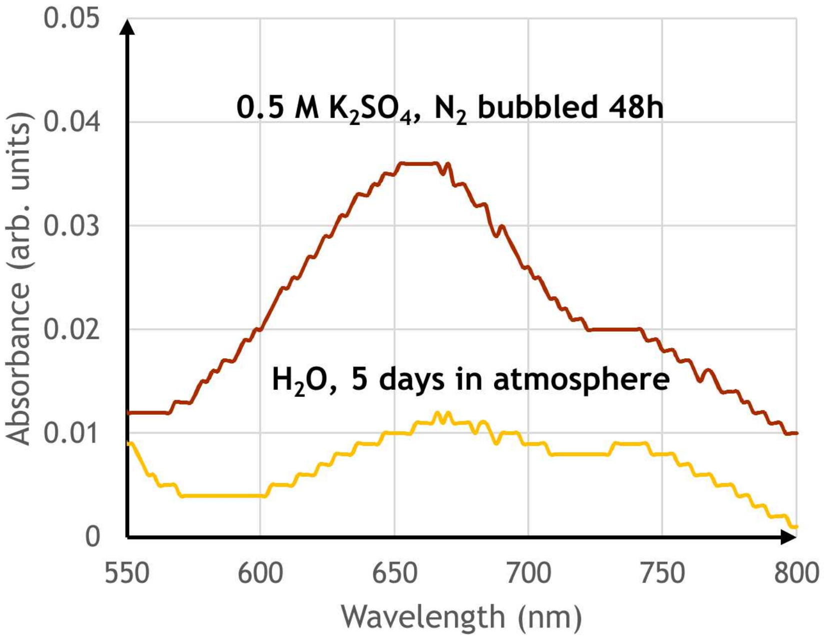
Endophenol colormetric confirmation

Differential Electrochem Mass Spec sampling

N15 method as needed

Detecting NH3 can be tricky





- **Ammonia from vial caps**
  Water soaked in vial caps for 1h
  Water in vial: trace NH_3
  Black cap: 0.003 mM of NH_3
  White cap: 0.009 mM of NH_3

- **Ammonia from atmosphere**
  Electrolyte N_2 bubbled for 48 hours
  : 0.003 mM of NH_3
  Water left in atmosphere for 5 days
  : trace NH_3

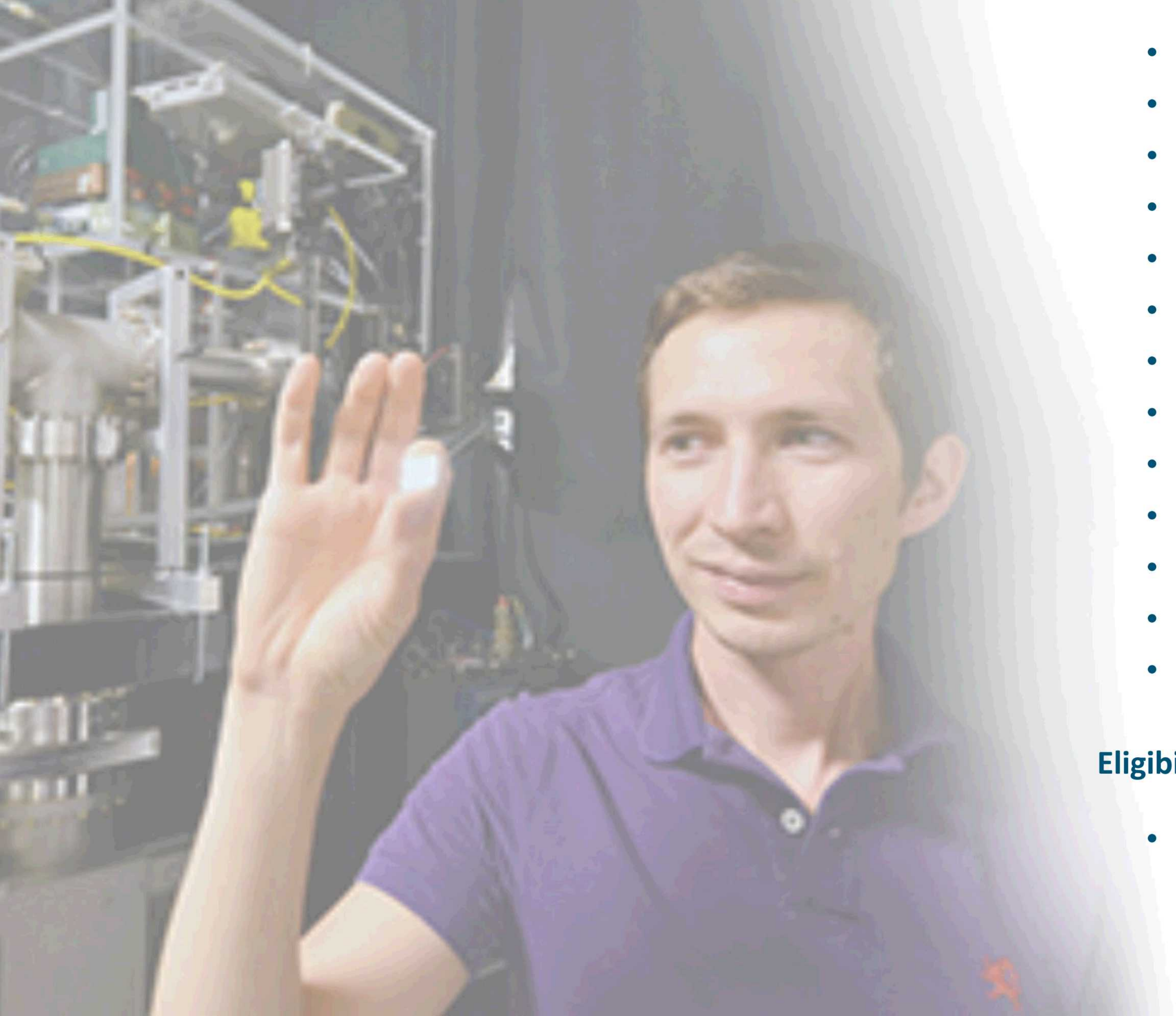
Internships

Encourages qualified students to develop interests in critical skills areas related to our mission, with the ultimate objective of developing our pipeline for our future. Available for Summer, Year Round and Co-op.

Eligibility Criteria

- Full-time enrollment status at an accredited school during the academic school year
- Undergraduate equivalent of 12 hours per semester
- Graduate equivalent of 9 hours per semester
- Must have a minimum cumulative GPA of 3.0 on a 4.0 scale for Technical, R&D, and Business interns; 2.5 on a 4.0 scale for Clerical and Labor interns
- Have U.S. citizenship for positions that require a security clearance or as stated in the job posting
- At least 16 years of age

Post-doc Opportunities



Key areas for post-docs at Sandia:

- Computer science/Computer Engineering
- Electrical Engineering
- Mechanical Engineering
- High-performance computing
- Microelectronics and microfluidics
- Nanotechnology
- Physics
- Chemistry/ Electro Chem
- Biosciences and biotechnology
- Radiation & electrical sciences
- Engineering sciences
- Pulsed power sciences
- Materials science & engineering

Eligibility Criteria

- A recent PhD (conferred 5 years prior to employment) or the ability to complete all PhD requirements before hire date.

Fellowship Opportunities

Sandia provides postdoctoral fellows with professional development opportunities and prepares fellows to conduct independent, groundbreaking research.

Postdoctoral Fellowships

- Harry S. Truman Fellowship
- Jill Hruby Fellowship
- John Von Neumann

**Sign up for Automated Job Notifications!*

Veterans

Recognizing that veteran capabilities and attributes complement our mission and values, we're intent on attracting the nation's top veteran talent to our company.

At Sandia, you'll find qualities and features that sustain your dedication to being part of something bigger:

- A work ethic and environment driven by a critical mission
- Career possibilities in an array of fields that support national security, such as engineering, biosciences, energy research, cybersecurity, business and operational support, and more
- Opportunities to contribute as an individual or in a leadership position

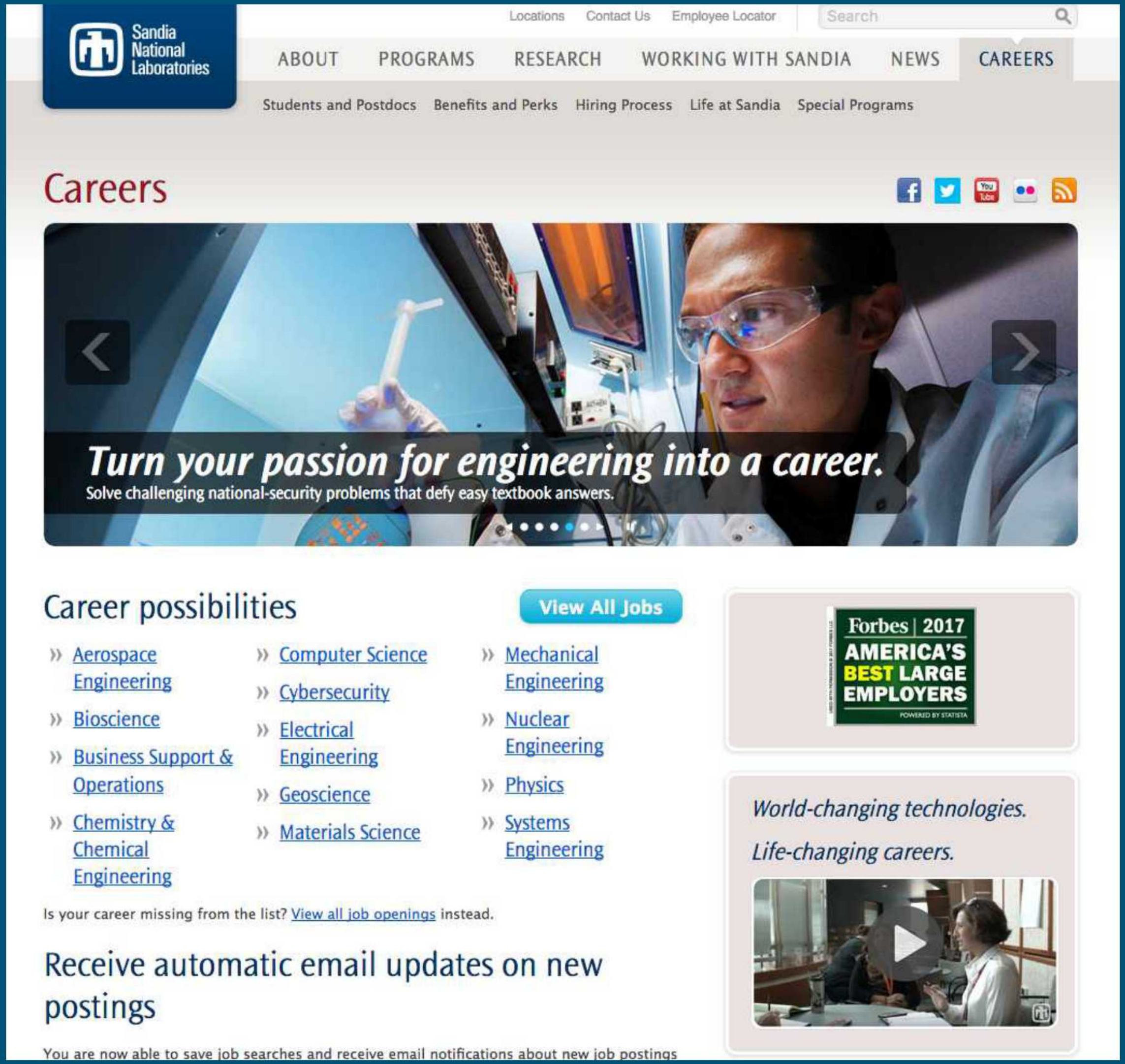
You'll also find encouragement to help you advance your career:

- Colleagues who respect and need your combination of experience and education
- Support, and possibly funding, to further your education
- The Wounded Warrior Career Development Program, which assists veterans with combat related injuries with employment, training, and education for a smooth transition to a civilian career

  Visit: www.sandia.gov Keyword search "**Wounded Warrior**"

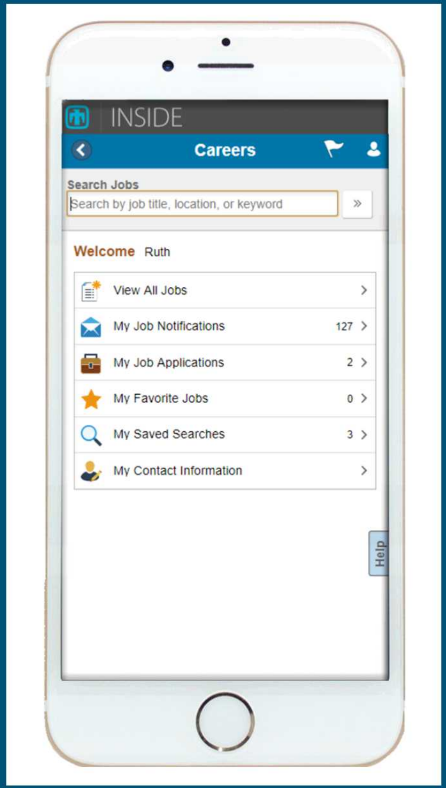
Sandia's Weapon Intern Program

Apply Online! sandia.gov/careers



Sign up for Automated Job Notifications!

Mobile Job Applications



Exceptional service in the national interest

GLOBAL SECURITY

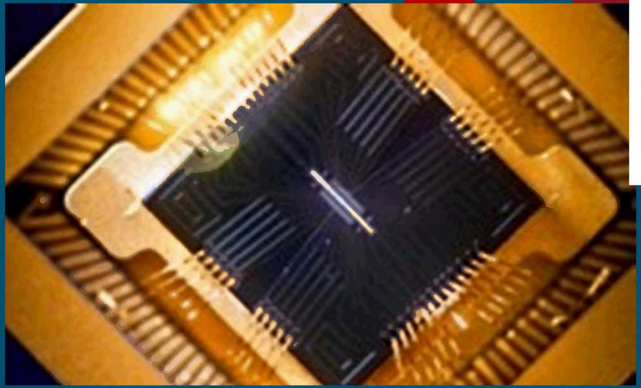
Protects the nation from threats at home and abroad

- Develop space- and ground-based sensor systems for monitoring emerging threats
- Supply technology, crisis response, and training to respond to a crisis associated with weapons of mass destruction
- Provide capabilities for protecting U.S. nuclear weapons and materials at fixed sites and in transit
- Produce systems that deter proliferation and verify compliance with international agreements using space-borne and ground-based sensing technology
- Lead global technical engagement to prevent the misuse of nuclear, chemical, biological, and radiological materials

NATIONAL SECURITY PROGRAMS

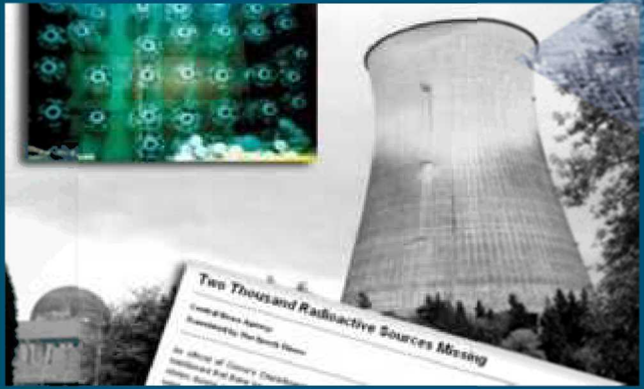
Strengthens our nation's defenders

Information operations



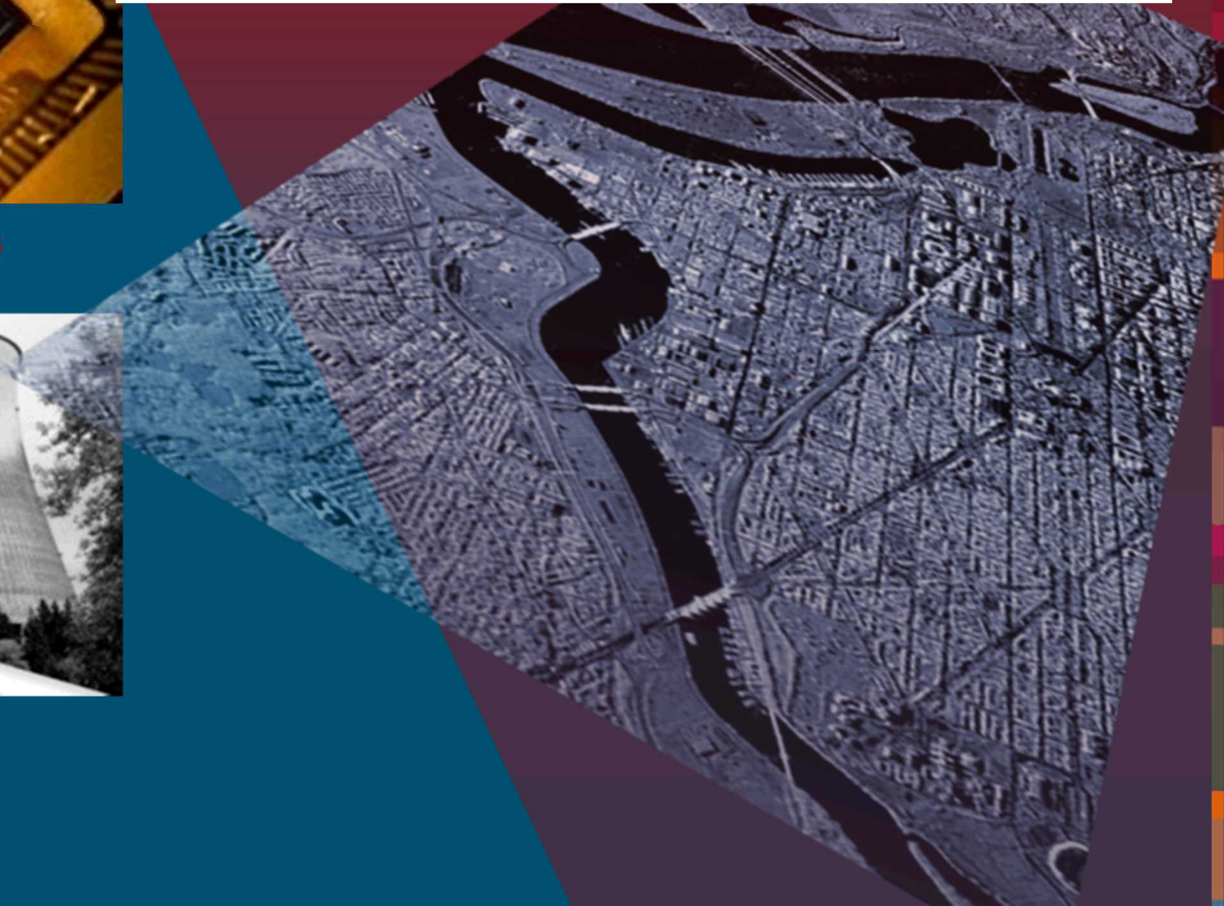
Science & technology products

Integrated military systems



Proliferation assessment

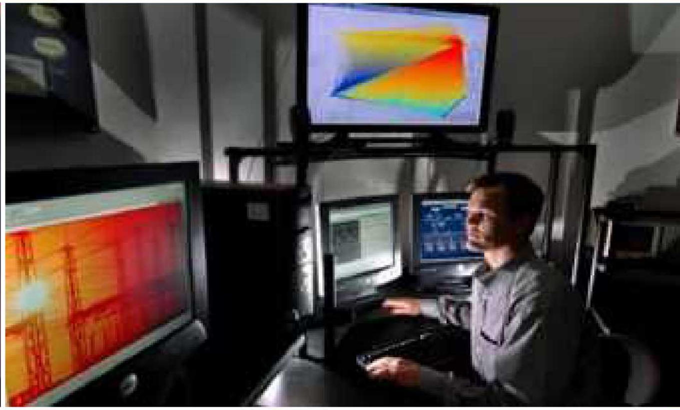
Surveillance &



ENERGY & HOMELAND SECURITY

Innovates for a secure future

- Perform fundamental and applied R&D to support the resilience and security of the nation's energy system
- Provide protection for our nation's digital and physical critical infrastructures
- Reduce U.S. vulnerability to chemical, biological, radiological, and nuclear threats
- Accelerate transformative innovations in the transportation sector through foundational physical and computational research



ADVANCED SCIENCE & TECHNOLOGY

Integrates multidisciplinary efforts to advance the science of the possible for Sandia's missions

WEAPONS SCIENCE & TECHNOLOGY

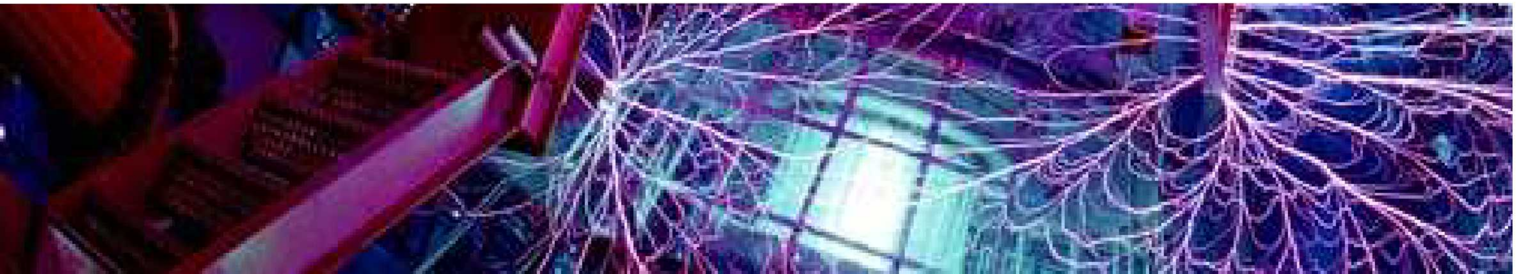
Provides Sandia with foundational science and engineering capabilities to ensure the nation's nuclear stockpile is safe, secure, and effective

OFFICE OF SCIENCE

Leads creative, hypothesis-driven inquiry in fundamental science to promote national security and international scientific leadership

CHIEF RESEARCH OFFICER

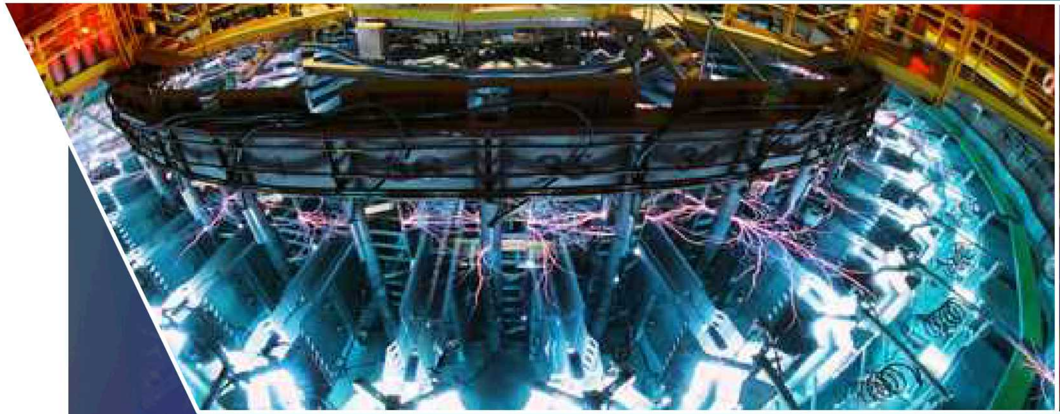
Governs and leads research strategy and stewardship of capabilities at Sandia, including the Laboratory Directed Research and Development program. Responsible for leadership of technology transfer and Sandia's partnerships with universities, industry, and the state of New Mexico.



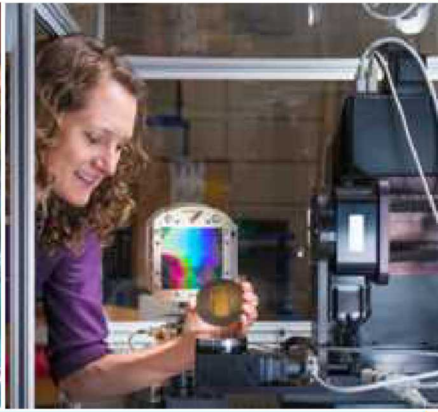
ADVANCED SCIENCE & TECHNOLOGY

Resear… ral role in mission delivery

Nanodevices & Microsystems

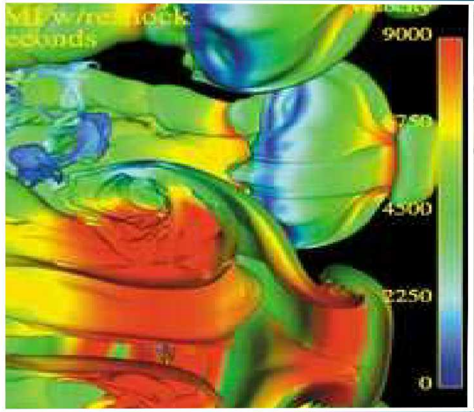


Radiation Effects & High Energy Density Science



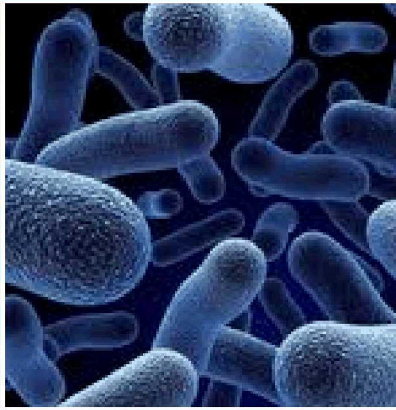
Materials Science

Computing & Informa



Engineering Science

Geoscience



Bioscience

VE IT. SANDIA'S MANY DISCIPLINES HER TO DO AMAZING THINGS.

Our science and engineering expertise produces technologies that change the world

RADIATION-HARDENED COMPONENTS

The Galileo spacecraft survi
Jupiter's radiation belts bec
of rad-hard components
designed and built by Sanc

HIGH-TECH PARACHUTE

Parachute technology designed for nuclear weapons helped the Pathfinder spacecraft bounce and roll when it hit the surface of Mars

SNYTHETIC APERTURE RADAR

Copperhead, a SAR system, has saved the lives of countless servicemen and women by detecting IEDs from unmanned aerial vehicles

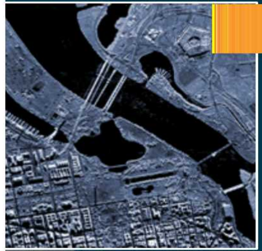
ESE CAPABILITIES MADE IT HAPPEN

RADIATION-HARDENED COMPONENTS

- Radiation Effects and High Energy Density Physics
- Materials Science & Engineering, and Advanced Manufacturing
- Physical and Biological Sciences and Engineering
- Codes, Models, Data Analytics
- Advanced Experimental Diagnostics and Sensors
- Agile Component and System Surveillance and Assessment

PARACHUTE TECHNOLOGY

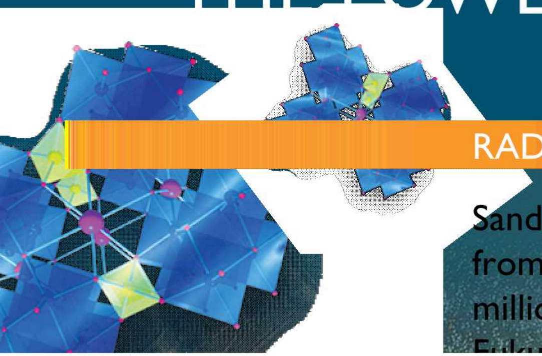
- Engineering Sciences and Testing
- Codes, Models, Data Analytics
- High Performance Computing
- Cyber and Intelligence Science
- Synergistic Global Security Engineering



SYNTHETIC APERTURE RADAR

- Materials Science & Engineering, and Advanced Manufacturing
- Physical and Biological Sciences and Engineering
- Codes, Models, Data Analytics
- High Performance Computing
- Agile Component and Systems Design, Engineering, and Integration
- Weapon Component and System Surveillance and Assessment

THE POWER OF MULTIDISCIPLINARY R&D SETS SANDIA APART



RADIOACTIVE WASTEWATER CLEAN UP

Sandia's method to remove radioactive contaminants from wastewater helped clean up more than 43 million gallons of contaminated water from Japan's Fukushima nuclear power plant.

OPERATION BURNT FROST

Our famous Red Storm computer helped the U.S. military intercept a defective spy satellite that threatened to fall to Earth in 2008. Using advanced modeling and simulation tools, we helped destroy the car-sized satellite traveling at 17,000 miles an hour with a single missile shot.

TRANSPORTATION ENERGY

Hydrogen fueling systems in Sandia's transportation energy research draw on our work in gas transfer that provides gas boosting for a nuclear weapon

THESE CAPABILITIES MADE IT HAPPEN

RADIOACTIVE WASTEWATER CLEAN UP

- Radiation Effects and High Energy Density Sciences
- Materials Science & Engineering, and Advanced Manufacturing
- Physical and Biological Sciences and Engineering
- Advanced Experimental Diagnostics and Sensors
- Agile Component & System Design, Engineering, and Integration

OPERATION BURNT FROST

- Engineering Sciences and Testing
- Codes, Models, Data Analytics
- High Performance Computing
- Cyber and Intelligence Science
- Synergistic Global Security Engineering

TRANSPORTATION ENERGY RESEARCH

- Materials Science & Engineering, and Advanced Manufacturing
- Physical and Biological Sciences and Engineering
- Codes, Models, Data Analytics
- High Performance Computing
- Weapon Component and System Surveillance and Assessment

WE DELIVER ON OUR NATIONAL SECURITY MISSIONS AND TOUCH LIVES EVERY DAY

CLEAN ROOM

Sandia pioneered clean room technology to protect the circuitry that controls nuclear weapons. It went on to be used in hospitals, for computers, and smartphones.

SENSOR TECHNOLOGY

Sensors developed to detect the acceleration pattern of warheads were an early component of automobile airbags

PREVENTIVE DETECTION

Teams from Sandia's Radiological Assistance Program are part of a national program that sends experts to large public events to scan the crowd for potentially harmful materials

THESE CAPABILITIES MADE IT HAPPEN

CLEAN ROOM TECHNOLOGY

- Microsystems R&D and Manufacturing
- Physical and Biological Sciences and Engineering
- Agile Component & System Design, Engineering, and Integration

SENSOR TECHNOLOGY

- Microsystems R&D and Manufacturing
- Engineering Science & Testing
- Materials Science & Engineering, and Advanced Manufacturing
- Codes, Models, Data Analytics
- Advanced Experimental Diagnostics & Sensors
- Energetic Materials and Components Science & Engineering
- Agile Component & System Design, Engineering, and Integration

PREVENTIVE DETECTION

- Radiation Effects and High Energy Density Sciences
- Advanced Experimental Diagnostics & Sensors
- Cyber and Intelligence Science
- Synergistic Global Security Engineering

[Nanoantenna Video](https://youtu.be/0i5zWgoxx1c) https://youtu.be/0i5zWgoxx1c

Available Videos

Videos require wifi in order to play

Sandia Mission Video (4:36)
Sandia Our Roots(3:05)

Location Videos
Sandia New Mexico Location (3:23)
Sandia California Location (3:41)

Diversity & Inclusion Videos
Black Leadership Outreach
Asian Leadership Outreach
American Indian Outreach
Hispanic Leadership Outreach

*For more Sandia Videos refer to Sandia's YouTube Channel