

Finding Your Way in Computational Electronic Structure

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Sandia National Laboratories

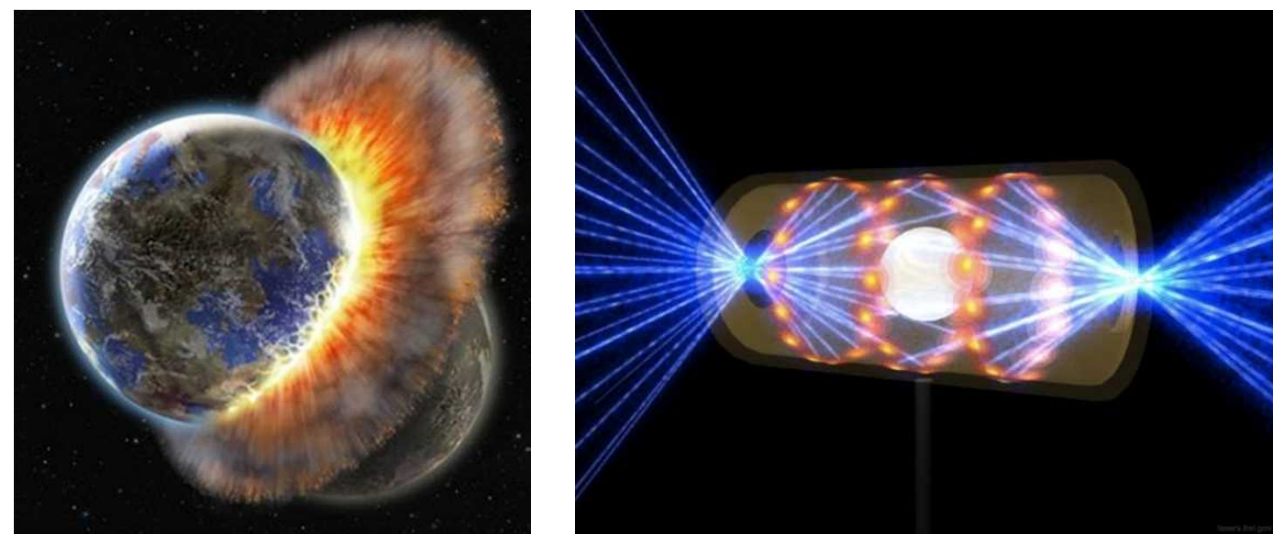
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While the results and impacts of electronic structure calculations seem ubiquitous, it takes a bit of an effort to develop a career in this field. With a background in density functional theory of chemistry and physics, I explored several opportunities before finding a fulfilling position investigating matter under extreme conditions. I will highlight my experiences working at several government labs (Los Alamos, NIST, and Sandia) and in industry (Philip-Morris and Enig Associates). Emphasis will be placed on where computational science can make a useful impact.



My Work History

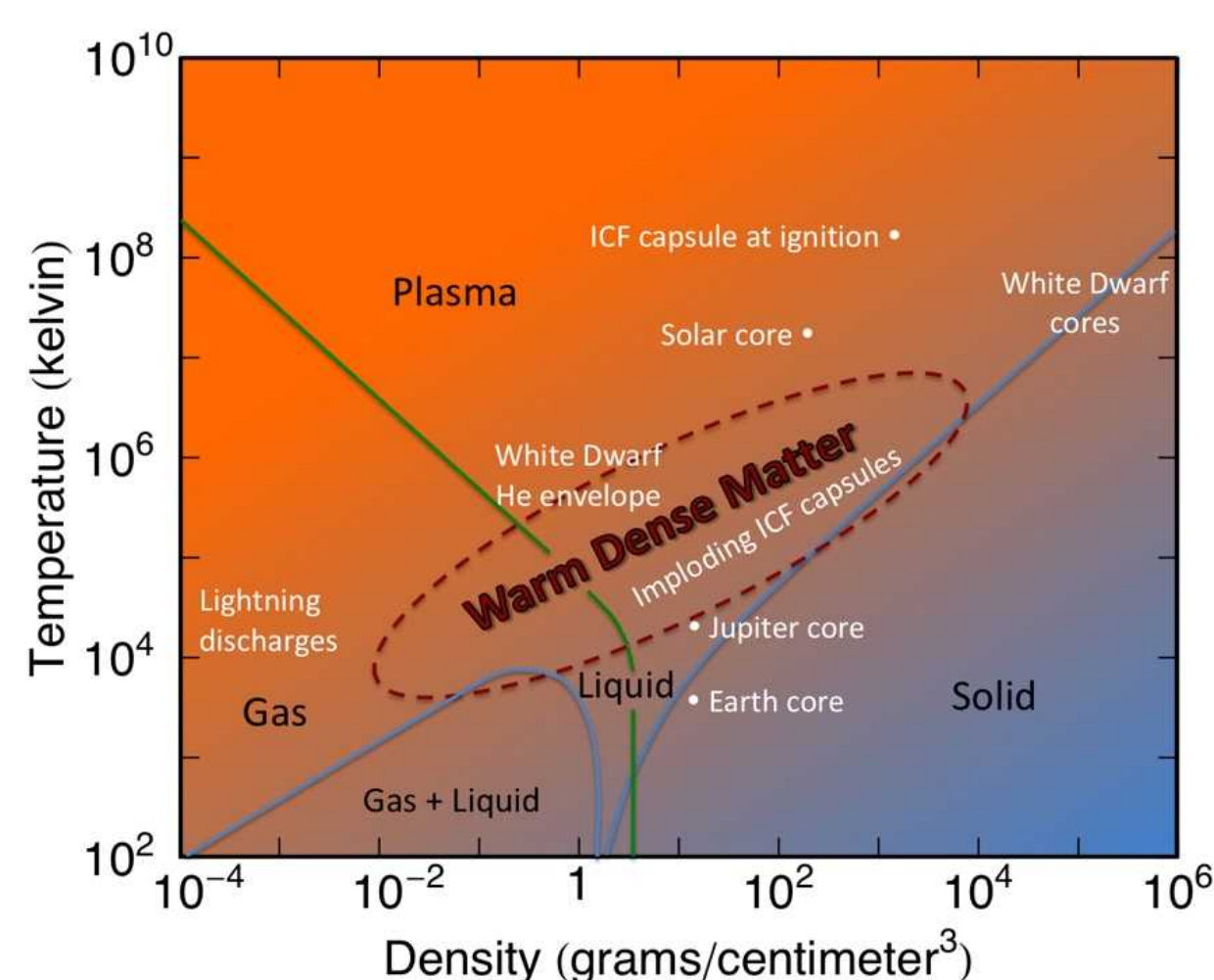
1. Los Alamos T Division Molecular Physics and Computational Chemistry
2. INEST at National Institute of Standards and Technology funded by Philip-Morris-USA
3. Enig Associates, Defense Contractor
4. Sandia National Laboratories



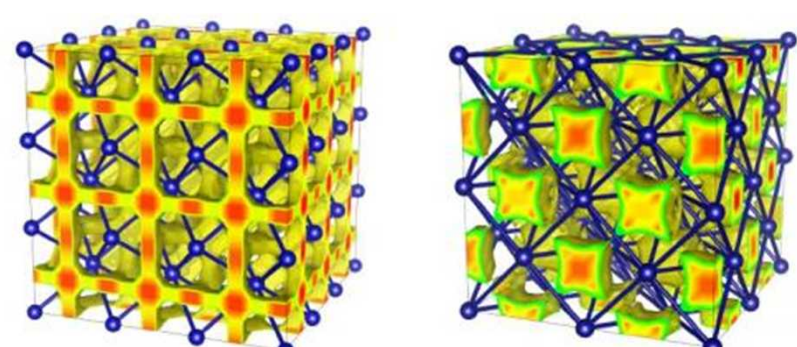
Materials Properties are Needed to Model Complex Phenomena through Equations of State.

- Pressure, density, temperature, phase....
- Materials science
 - Planetary collision science
 - Geoscience
 - Inertial confinement fusion

A Difficult Region of Phase Space to Access is the Warm Dense Matter Region.



- Highly compressed matter
- Temperature 10s of kK
- Accessible to experiment and theory
- Mbars of pressure



Super ionic water

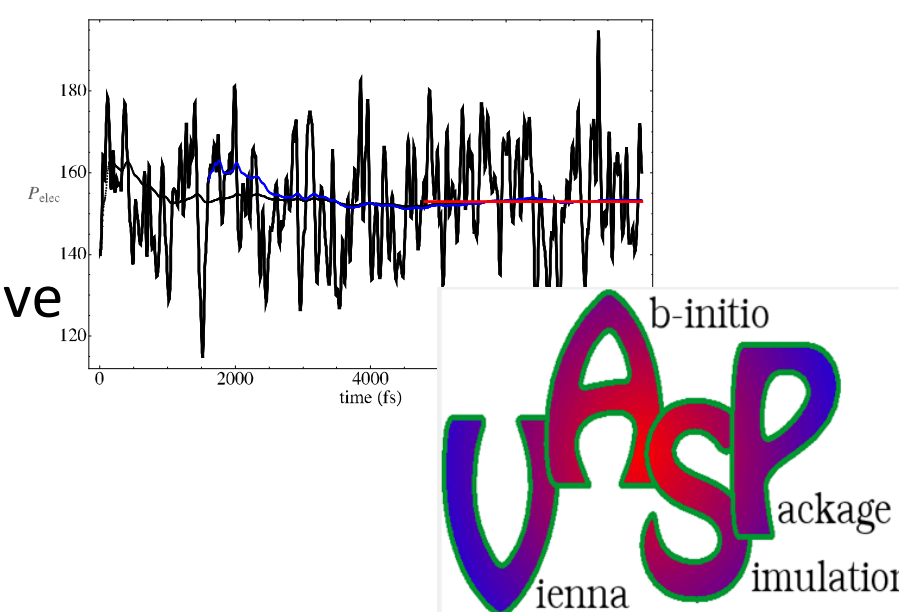
The Z-Machine can Probe this Region.

- The world's most powerful pulsed power machine
- Accelerates aluminum flyer plates to 40 km/sec.
- Delivers 27 MegaAmps in 95 nanoseconds.
- Achieves Pressures greater than 10 Mbar (1 TPa).
- Recent work on Xenon reached a state 840 GPa and 149kK
- Compare to diamond Anvil cell – up to 300 GPa and several kK
- Indirectly but Accurately Measures Pressures and Densities

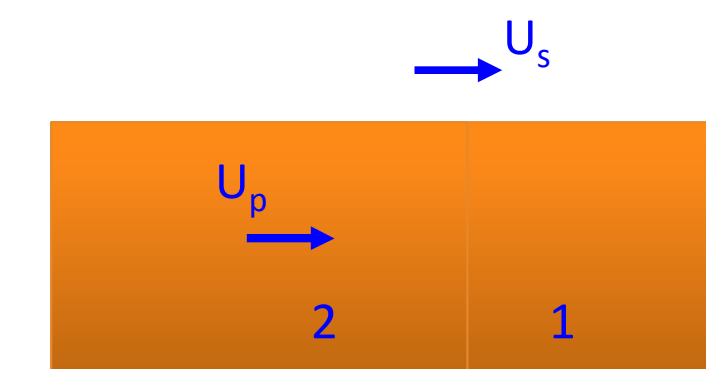
First Principles Probes

Density functional molecular dynamics (MD) simulations give thermo-physical properties

Unbiased as to elemental species

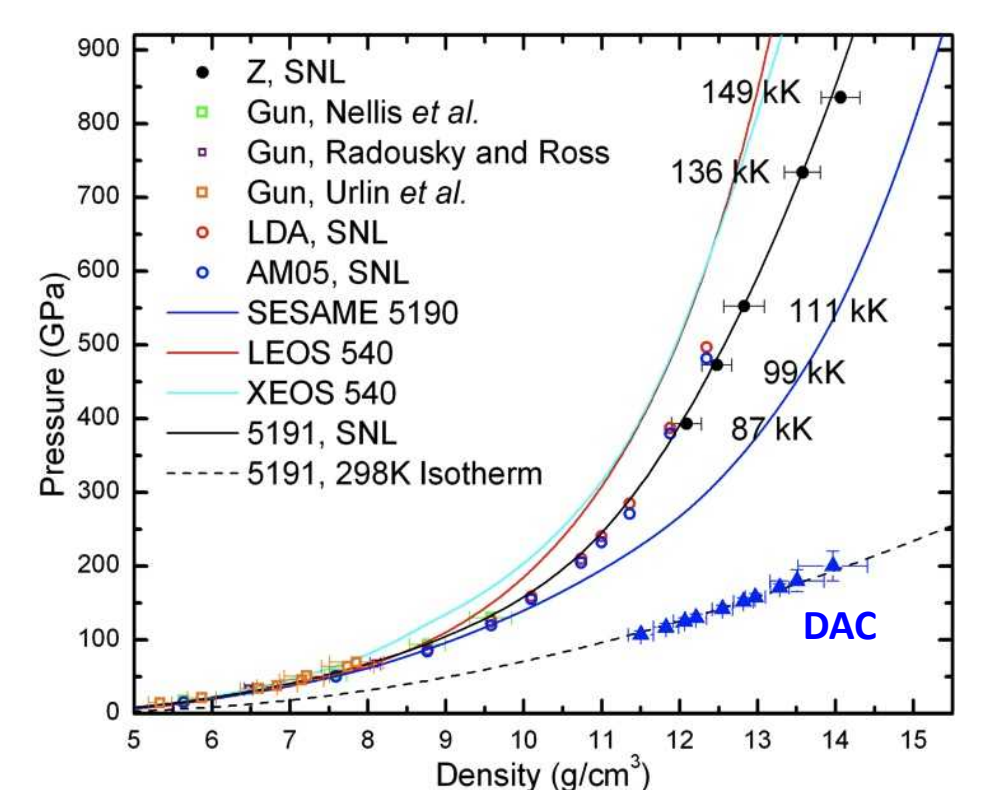


Conservation of mass, energy, and momentum lead to the Rankine-Hugoniot condition for the initial (1) and final state (2).
High accuracy measurement and/or calculations of thermo-physical properties can be compared to validate understanding.



$$2(E_2 - E_1) = (P_2 + P_1)(v_1 - v_2)$$

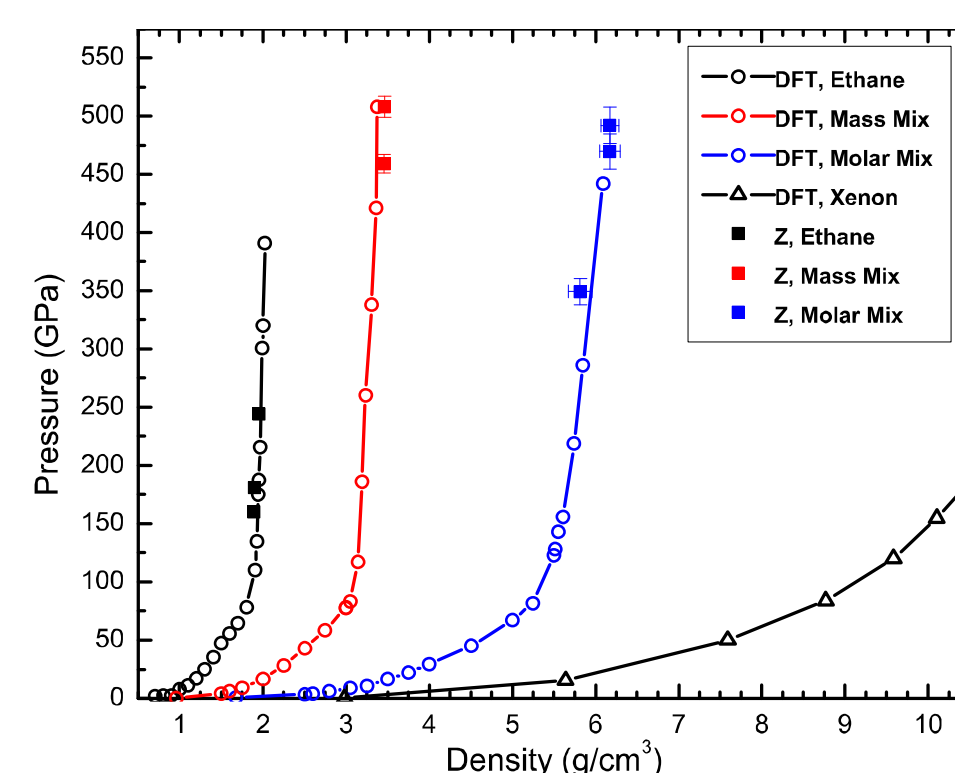
Experiments on Sandia's Z Machine Obtained High-Precision Data for Xenon to 840 GPa/ 14 g/cm³



Xe and Ethane

T=163.5 K, $\rho=1.5$ and 1.7 g/cm^3 , P=0 GPa, Molar mix ratios 42% and 50%

Xe-Ethane (C_2H_6) Mix Hugoniot



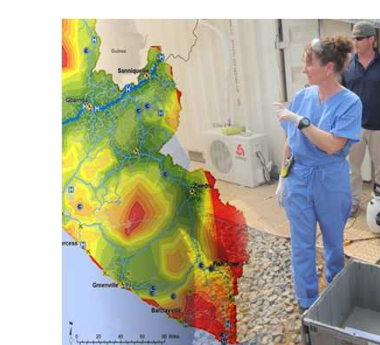
RJM and others, Phys. Rev. B **91**, 134109 (2015)

Sandia - Today

As a multi-faceted national security laboratory, Sandia has delivered essential science and technology for more than 60 years and plays a critical role in ensuring U.S. technical superiority.

At Sandia, you can become part of something more—and contribute to our quest to render exceptional service in the national interest.

Sandia's Impact



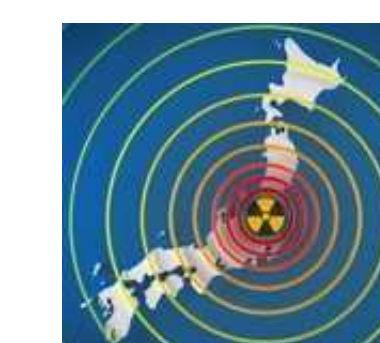
Ebola Outbreak

Ebola contributes to global response of Ebola outbreak by developing a sample delivery system cutting the wait time and potentially fatal exposure.



Cleanroom invented 1963

\$50 billion worth of cleanrooms built worldwide. It's used in hospitals, laboratories and manufacturing plants today.



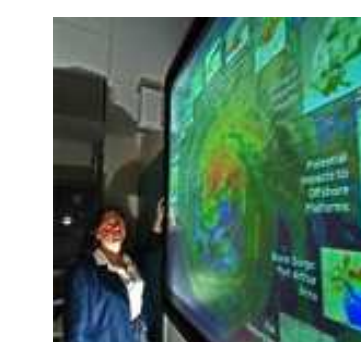
Fukushima Quake

Sandia helps clean up radioactive wastewater.



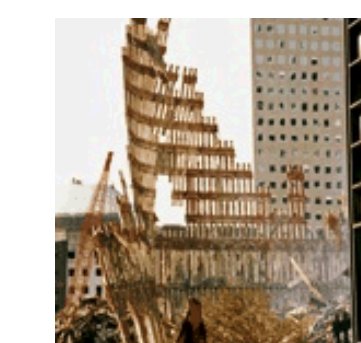
Detecting IEDs

Combat personnel now have a new tool for uncovering improvised explosive devices: Sandia's highly modified miniature synthetic aperture radar system, which is being transferred to the U.S. Army.



Hurricane Katrina

Sandia is called to assess flooding and infrastructure failures.

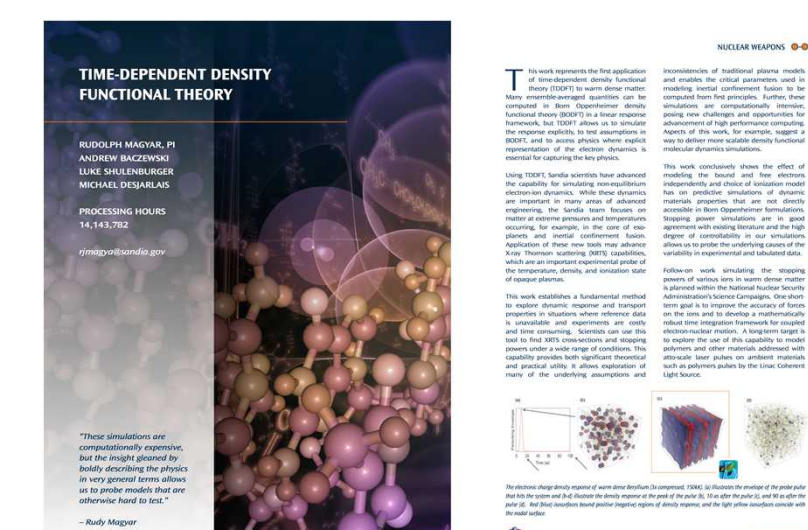


9/11

Sandia sets contingency plans for release of materials and aircraft attacks on critical facilities immediately after 9/11. Search dogs are equipped with cameras for search and rescue K-9 handlers. The capability allowed search efforts to be carried out in spaces inaccessible to humans.

My Experience at a Lab

1. Interesting work
2. Great and talented coworkers
3. Fundamental as well as applied research
4. LDRD
5. Opportunity to attend conferences
6. Flexibility
7. Compensation



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.



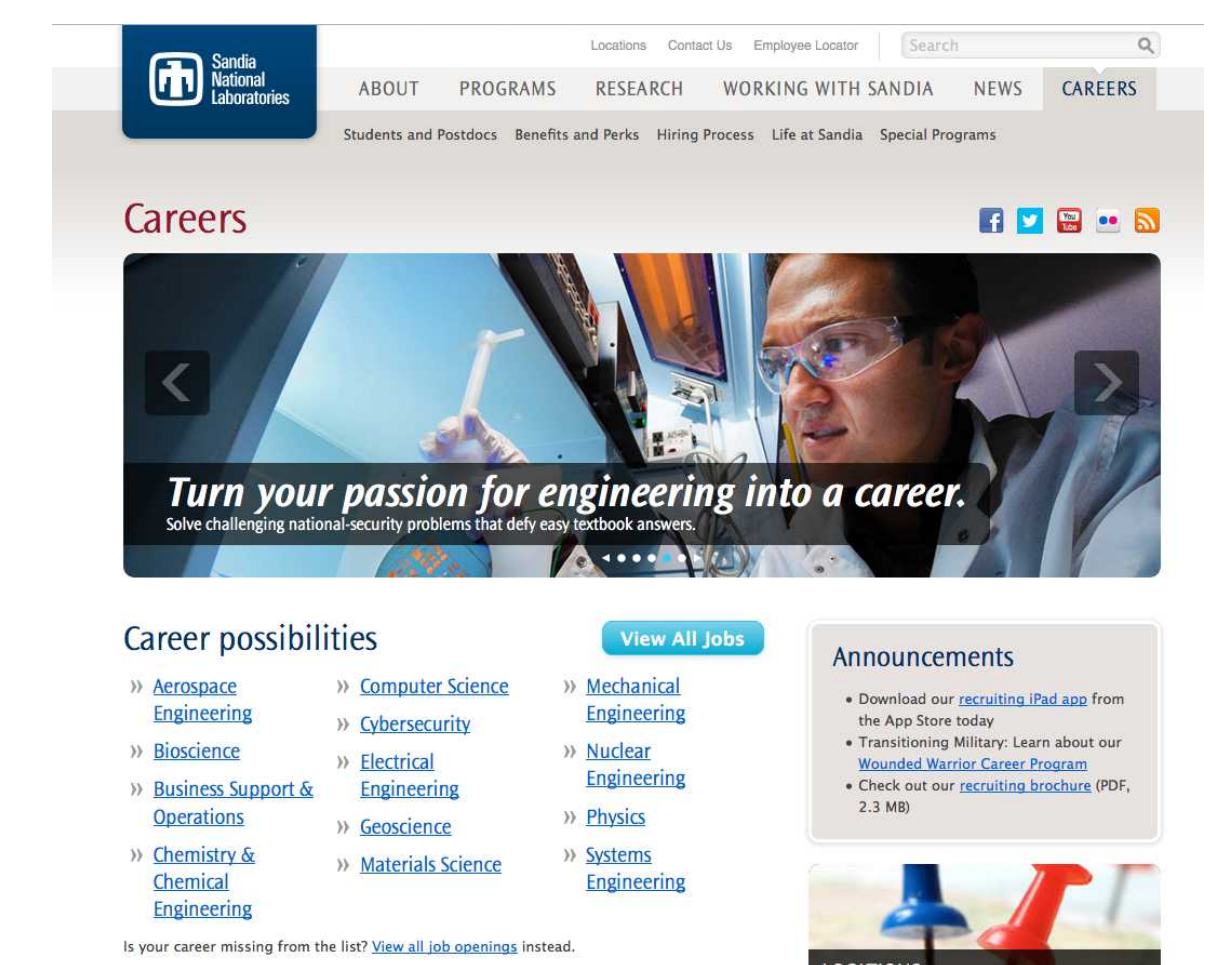
Post-doc Opportunities

Key areas for post-docs at Sandia:

- Biosciences and biotechnology
- Chemistry and materials science
- Combustion
- Computational mechanics
- Computer science
- Hydrogen
- Microelectronics and microfluidics
- Nanotechnology
- Physics

Eligibility Criteria

- A recent PhD (awarded within the past five years) or the ability to complete all PhD requirements before beginning
- No previous post-doc appointments at a national laboratory



sandia.gov/careers