Lawrence Livermore National Laboratory

Science and Technology on a Mission

Hydrogen and Fuel Cell Technical Advisory Committee

DOE- EERE, Fuel Cell Technology Office

April 7, 2016

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Director, Energy and Climate Security

Office of the Deputy Director for Science and Technology

Lawrence Livermore National Laboratory

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Lawrence Livermore National Laboratory

LLNL is a multidisciplinary national security laboratory

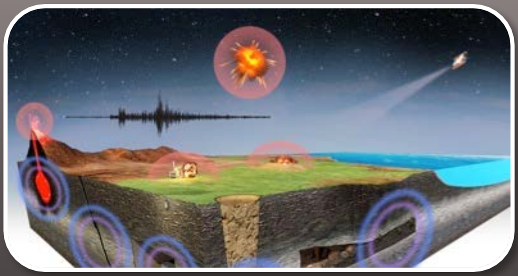
Experimental Test Site
(11 sq. mile site near Tracy, CA)

- Established in 1952
- Approximately 5,900 employees
- 1 square mile, 684 facilities
- Annual federal budget: ~ $1.53B

Solving global security challenges for the nation

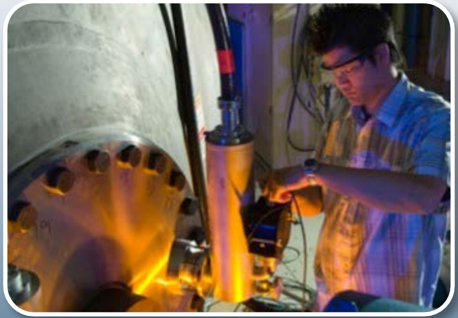
Multidisciplinary science, technology, and engineering

Nuclear Security



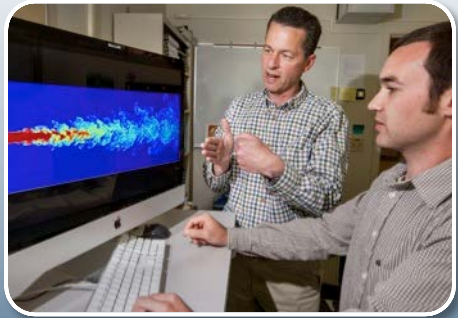
International and Domestic Security

Energy and Environmental Security



Science

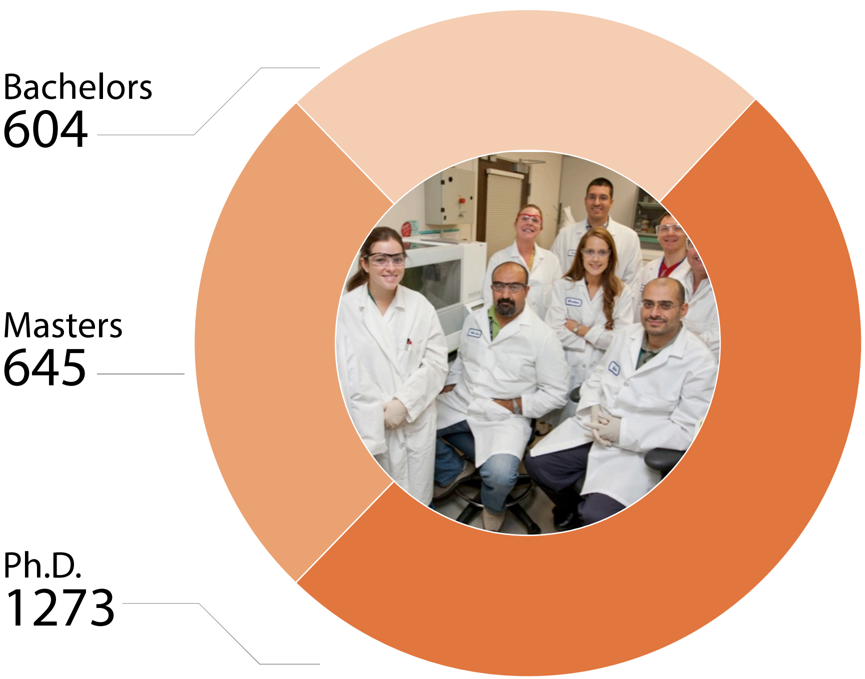
Engineering



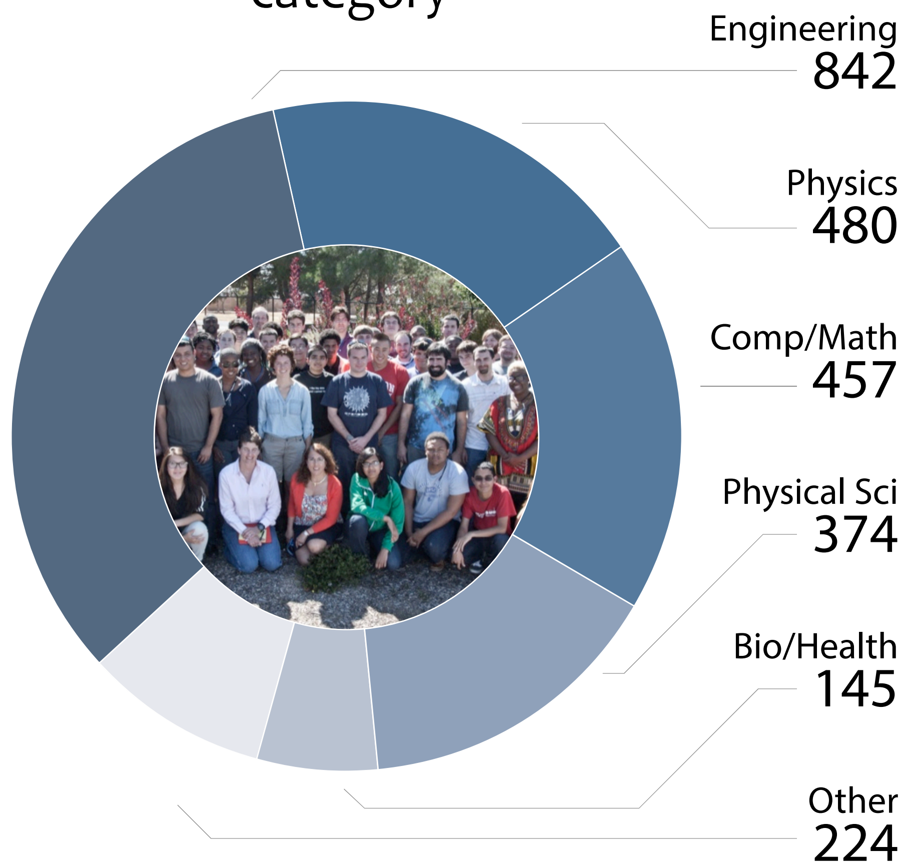
Computing

LLNL has a talented and multidisciplinary technical workforce

ST&E by highest degree



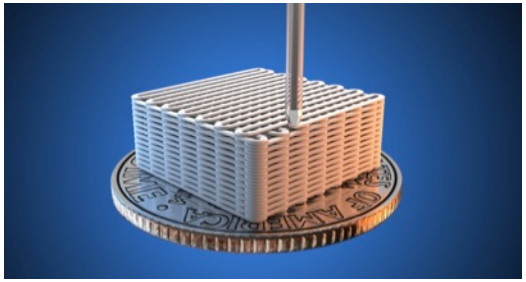
ST&E by degree category



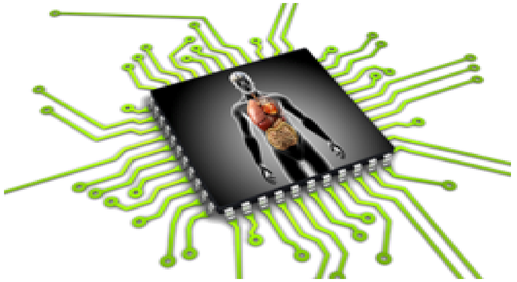
S&T Core Competencies

High-Energy-Density Science

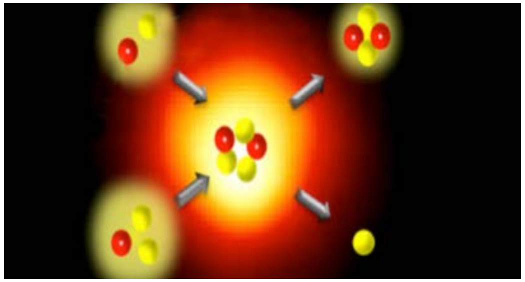
Advanced Materials and Manufacturing



Bioscience and Bioengineering

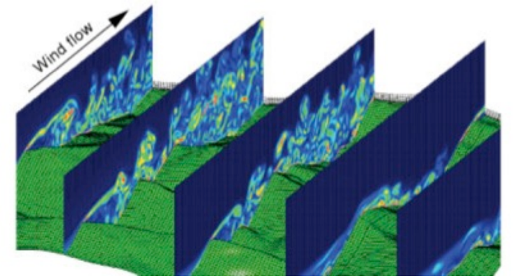


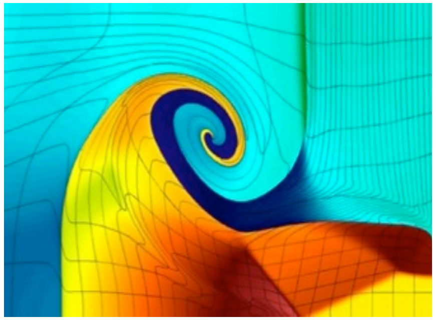
Nuclear, Chemical, and Isotopic S&T



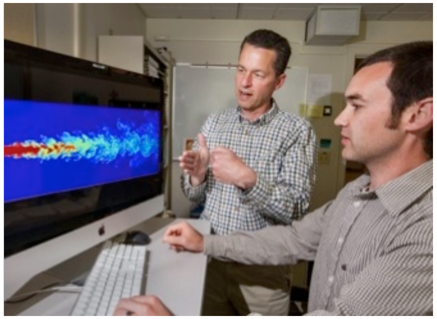
Lasers and Optical S&T

Earth and Atmospheric Science





High-Performance Computing, Simulation, and Data Science

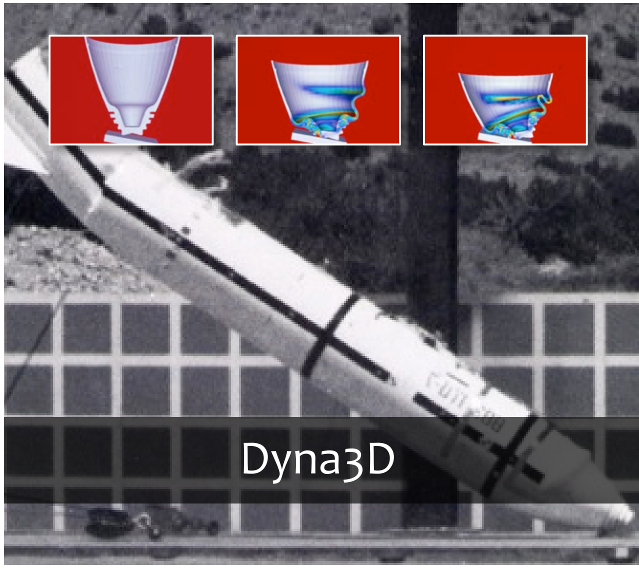


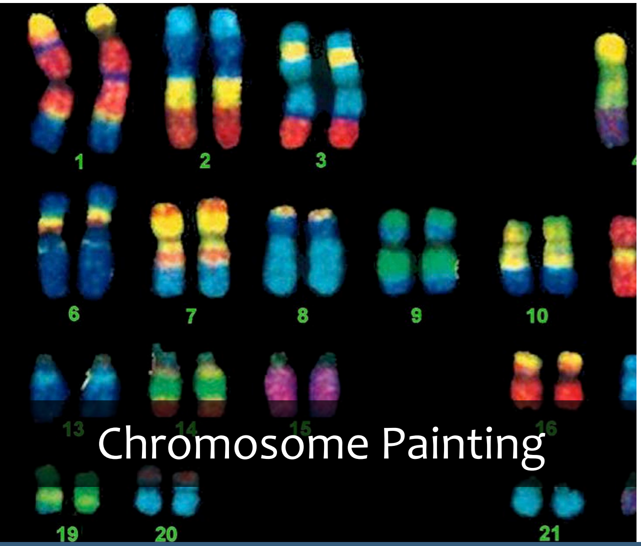
LLNL
Science, Technology, and Engineering

Real-world solutions


Plastic Radiation Detectors


Laser Peening


Dyna3D



Chromosome Painting


Artificial Retina

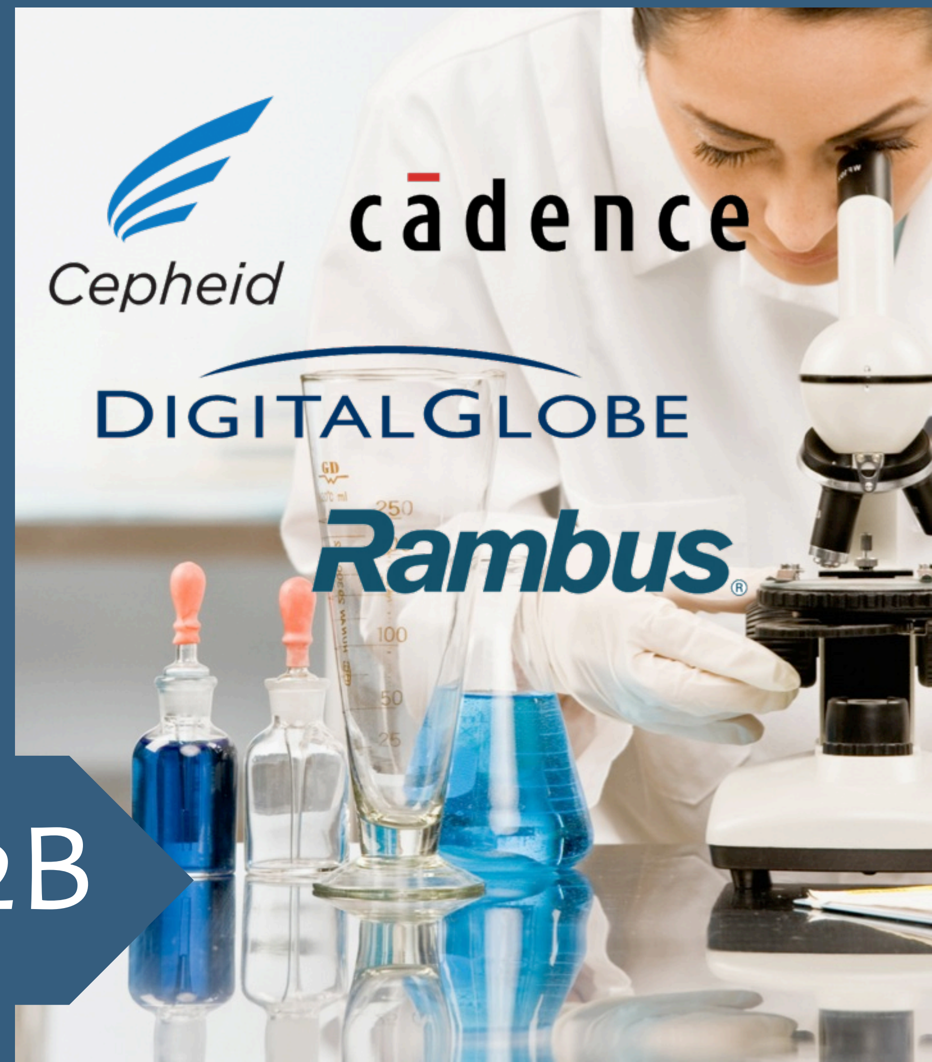

Microbial Detection Array

LLNL technology has transferred directly into the economy

$350M in goods and services were produced in 2015 using LLNL intellectual property

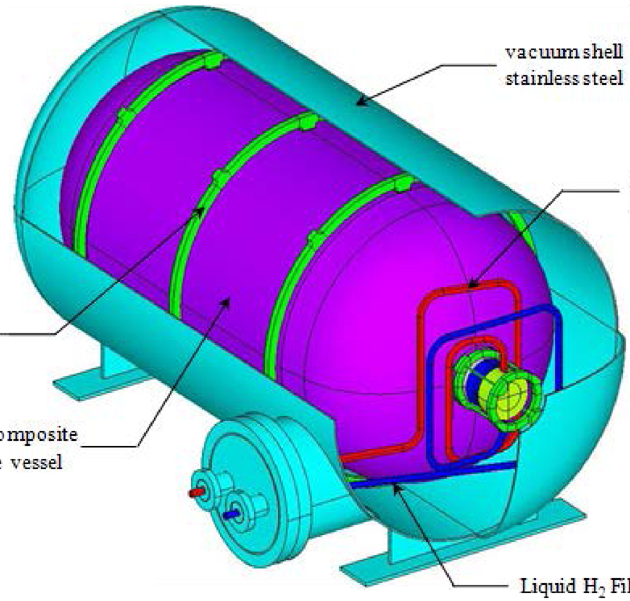
A three-year-old local startup, Quantalife, was sold in 2011 for more than **$162M**

Top four companies started by LLNL scientists have a market value of over **$12B**



LLNL is partnering with BMW to deploy cryo-compressed hydrogen automobiles

Safe, Long-Range, Cost Effective, Zero Emissions Transportation with Cryogenic Pressurized Hydrogen Storage and Delivery



Cryogenic pressure vessels have the best performance:

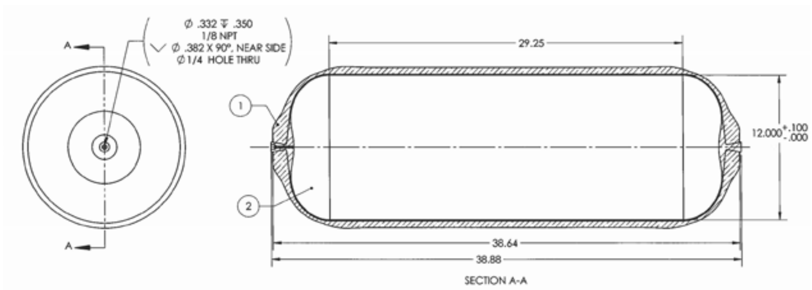
- Highest system storage density (43 g/L)
- Highest hydrogen weight fraction (7.5%)
- Lowest cost of ownership (Argonne)
- Compelling safety advantages:
  - 20X less expansion energy than 300 K gas
  - Inner vessel protected by vacuum jacket
  - Gas expansion into vacuum jacket reduces thrust by 10X

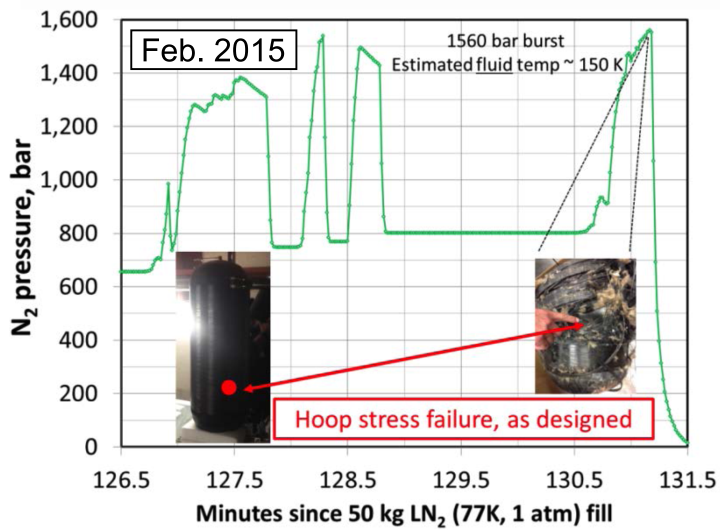
Outstanding issues:

- Scalability to smaller diameters (35 cm)
- Vacuum stability
- Manufacturability

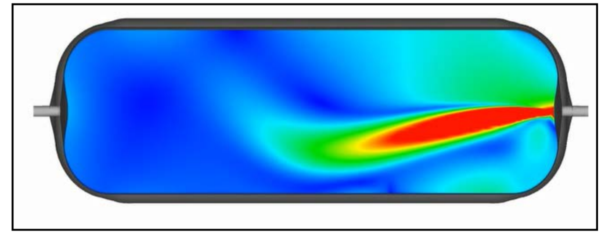
Cryogenic pressurized storage and delivery provide safety, cost and weight advantages over alternative approaches to long-range (500+ km) zero emissions transportation

In a CRADA with BMW, we are demonstrating durability of the most volumetrically efficient 700 bar pressure vessels ever built





First prototype cryo burst tested to 1560 bar



CFD and stress analysis performed by BMW AG

Vessel prototypes have had continuously improving cycle lives. To be soon cryogenically cycle tested

Goal: Develop and cycle durable, ultra-compact 700 bar cryogenic H_2 vessels
Target : 5 kg H_2 system with 9+ wt% & 50 g/L, demonstrating 1,500 cycles

We have built the most capable H_2 facility for cost effective cyclic, thermomechanical, permeation, leak, durability, and burst testing

- LH_2 pump (Linde) delivers rapid throughput (100 kgH_2/h)
  - 5 minute refueling of full-scale vessels
- 80 g/L fill density, double of 700 bar compressed H_2
- 3000 gallon Dewar sufficient for refueling 150 vehicles
- 3 m^3 containment vessel rated for 4 pounds TNT equivalent
  - enables testing of full scale vessels

Please contact us for all your hydrogen system testing needs

Detailed cost evaluation of cryogenic pressurized storage and delivery demands estimation of evaporative losses from all steps in the process

[A]* Dewar: 0.5 W/m^2. 5.5 kg/day for a 725 kg tank

[B] Lines : 1 W/m^2 (~10 cm diameter, 5 m length). 0.3 kg/day per line.

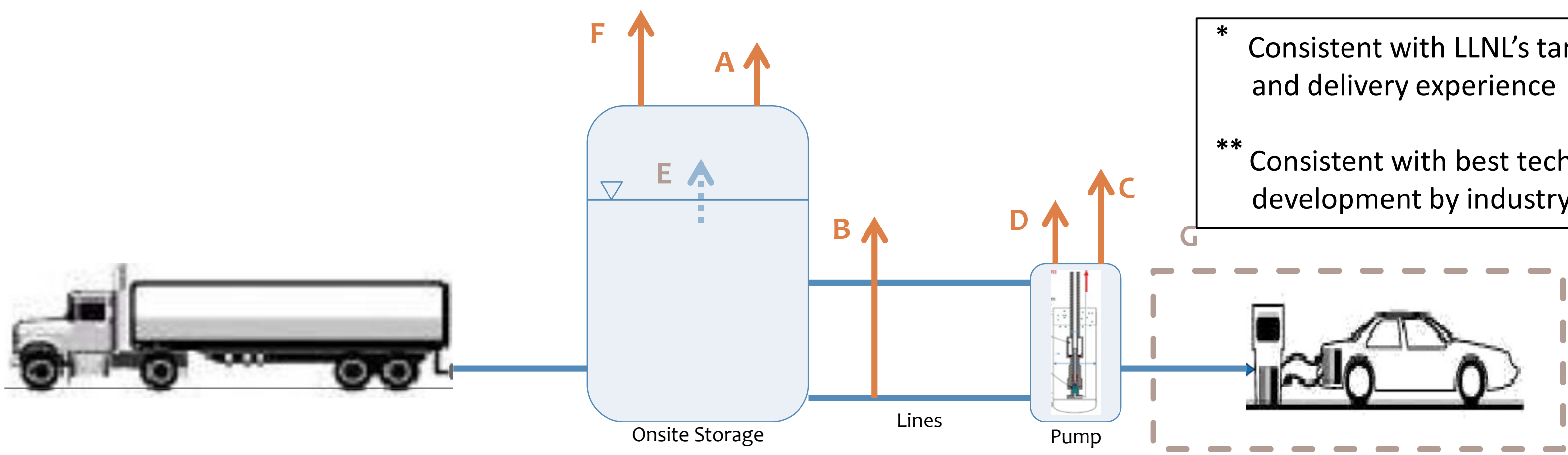
[C]** Pump: 0.5 W/m^2 over outer surface area of immersion dewar. 1.1 kg/day per pump.

[D]** Pumping: 0.03% of ideal pumping work (882 kJ/kg). 0.5 kg/day at 400 kg/day per pump.

[E] Avoided losses: 0.073 kg H_2 must be evaporated per kg H_2 dispensed.

[F]* Delivery losses: 4.2 kg H_2/m^3 headspace or 0.07 kg vented per kg-LH_2 delivered.

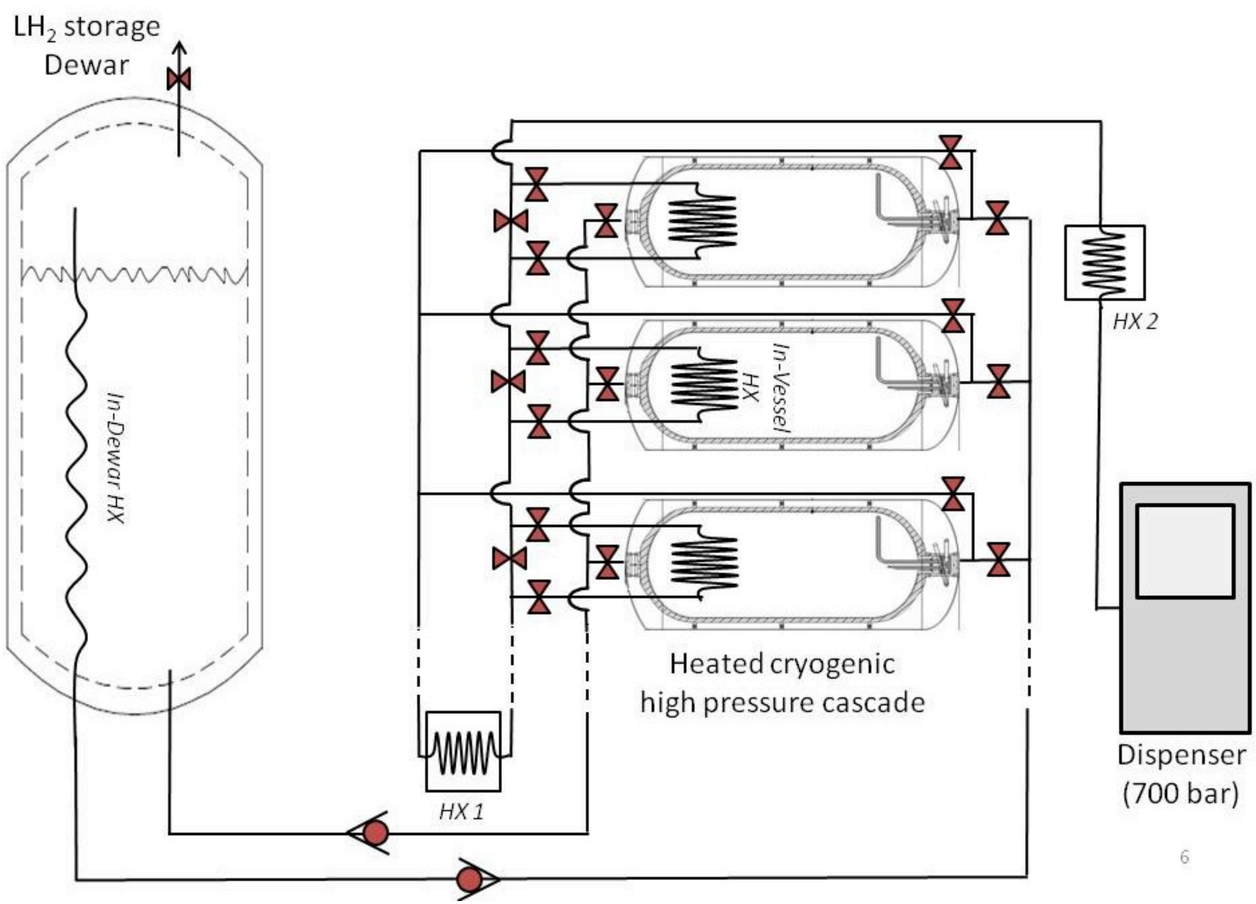
[G] Station-related losses from the high pressure section (lines, dispenser and vehicle) are assumed to be zero.



* Consistent with LLNL's tank operation and delivery experience

** Consistent with best technology in development by industry partners

Thermal compression leverages LLNL's LH_2 facilities and expertise to eliminate expensive and maintenance-prone



- Compressors are 60% of station cost
- Eliminate compressors with a cascade of insulated, cryogenic compatible vessels with judicious use of heat exchange between them
- Conduct modeling to evaluate cost advantages
- Demonstrate basic functionality in proof of concept experiment

Goal: Reduce 700 bar fueling station cost by eliminating compressors
Target : At least 15% lower H_2 dispensing cost compared to baseline

EERE HyMARC Consortium for all-solid-state hydrogen storage

As part of the HyMARC consortium, LLNL is developing **novel theory & characterization tools** and **foundational understanding** of thermodynamics and kinetics for future onboard solid-phase hydrogen storage

Motivation

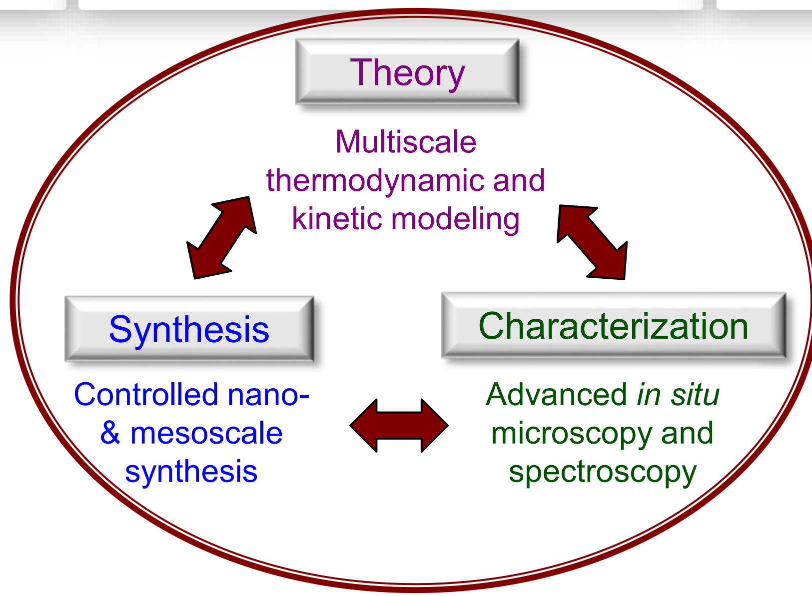
- Efficient and lightweight solid-state hydrogen storage would **revolutionize** fuel cell vehicles
- Need **better understanding** and **improved tools** to help the community develop new materials

Technology summary

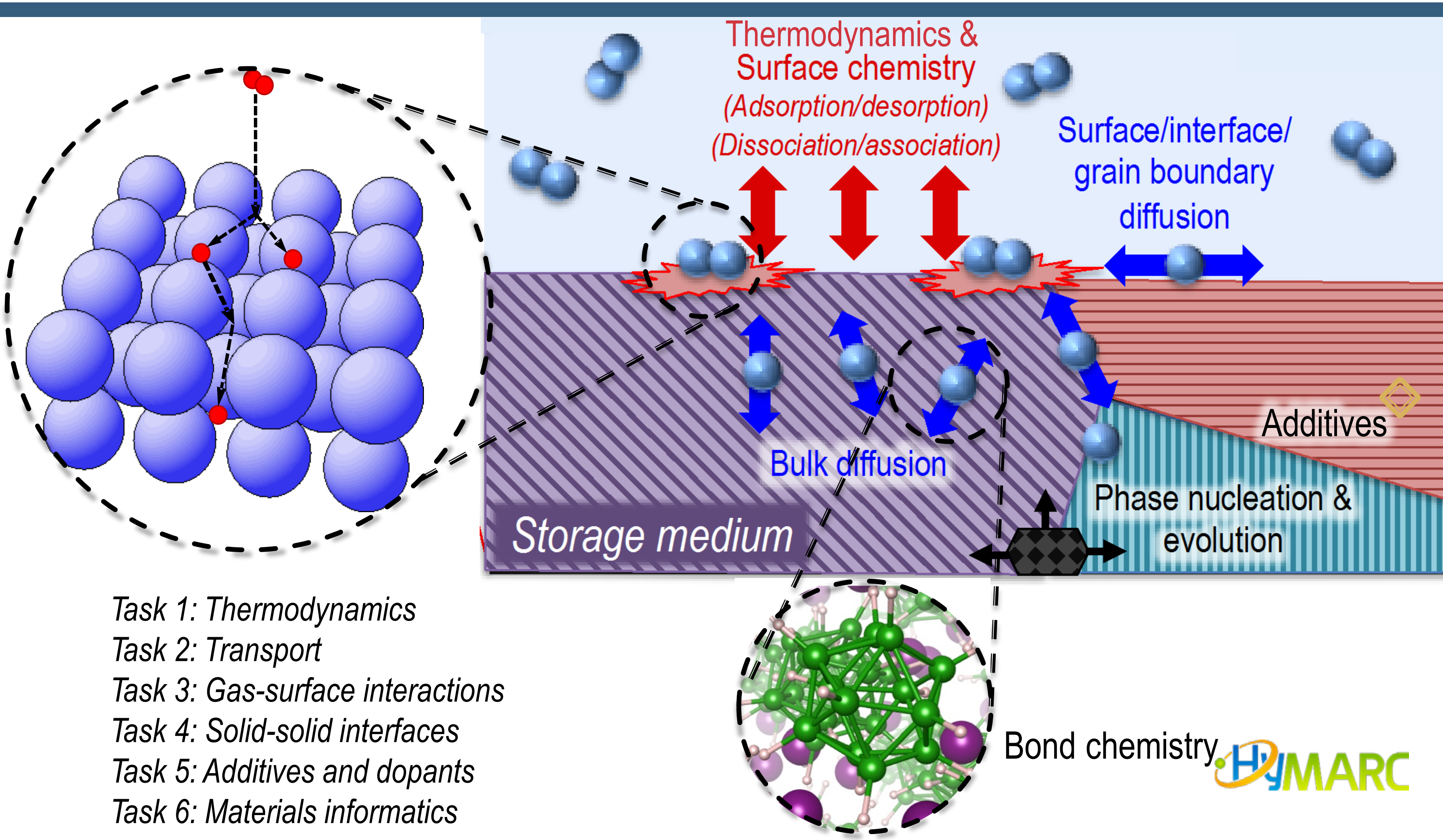
- LLNL brings expertise in **multiscale modeling, porous carbon synthesis, and *in situ* X-ray spectroscopy**
- Multiscale modeling focuses on understanding **"real" materials** during operation

Impact

- New **software**, **methodology**, **characterization** procedures, and **data management** tools
- New scientific understanding can be used to devise improvement strategies



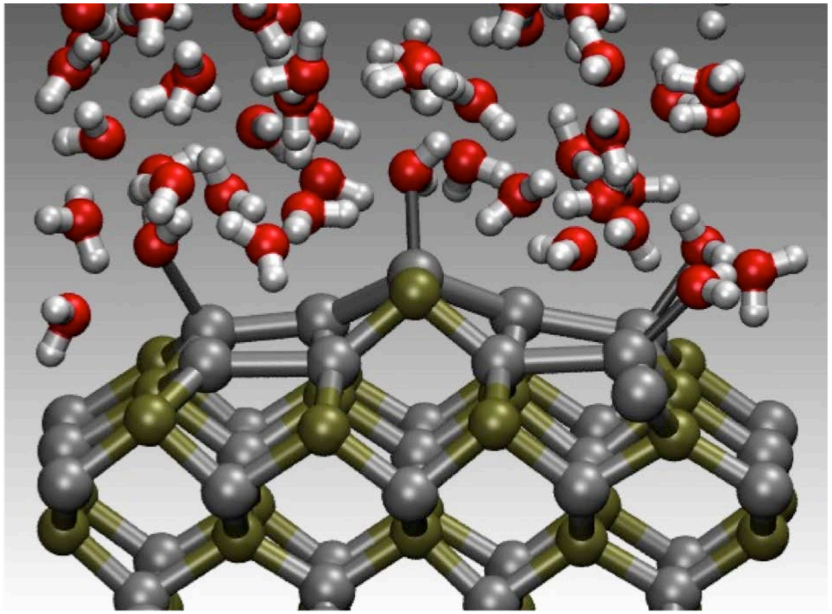
HyMARC tasks address thermodynamic and kinetic issues in solid-state H_2 storage



Task 1: Thermodynamics
Task 2: Transport
Task 3: Gas-surface interactions
Task 4: Solid-solid interfaces
Task 5: Additives and dopants
Task 6: Materials informatics

Solar photoelectrochemical H_2 production

- **Efficient and stable photoelectrochemical water splitting** requires solar absorbers, buffers, and surface layers with properly aligned band edge positions
- **Dual stacked absorber configurations** offer practical route to high solar-to-hydrogen (STH) efficiencies
- Use advanced theory to:
  - *Identify absorbers with necessary bandgaps and suitable buffer layer partners for favorable charge transport*
  - *Identify synthesis conditions to "tune" defect chemistry and optimize solar conversion efficiency*

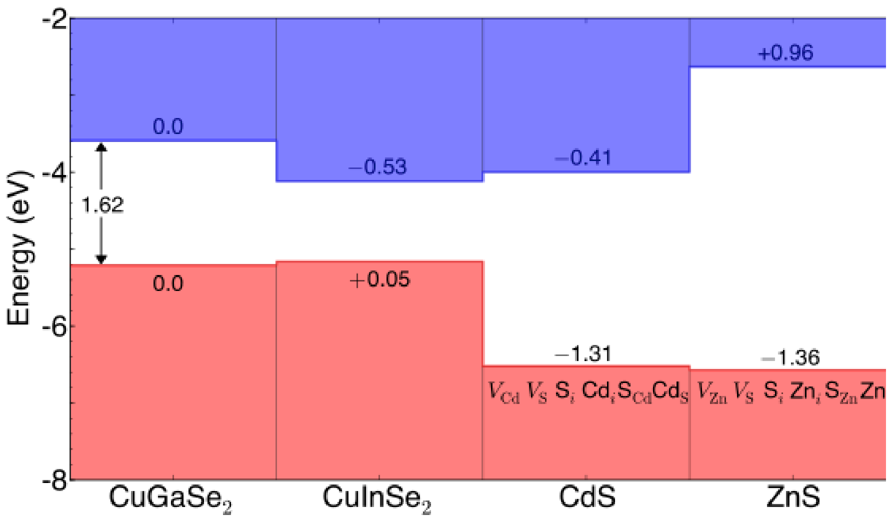


Interface between water and InP(001), a candidate material for solar photoelectrochemical hydrogen production

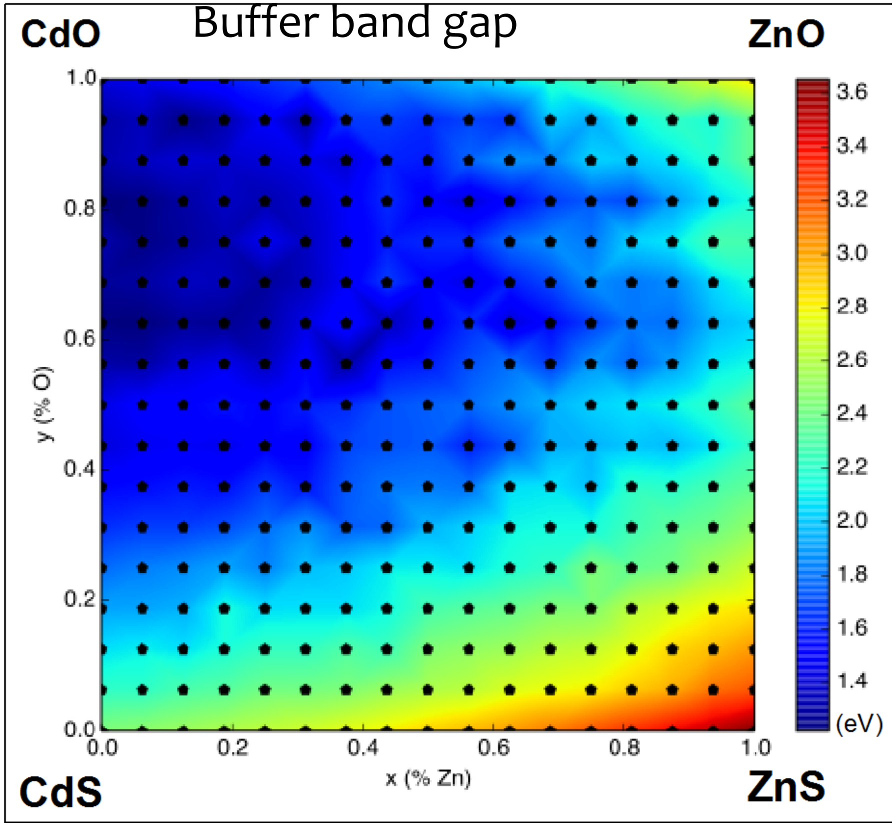
Solar photoelectrochemical H_2 production

- Optimal band gap of buffer must be slightly larger than photoabsorber
- Theory gives a recipe for choosing an optimal composition of oxide/sulfide buffer for each photoabsorber

Photoabsorber band gap



Buffer band gap



LLNL is playing leading roles on promising approaches to hydrogen production, delivery, and storage

- Cryogenic pressurized storage with 80% volumetrically efficient vessels promises safety and cost advantages with 50 gH_2/L, 9% H_2 weight fraction (BMW CRADA)
- LLNL hydrogen test facility enables cost effective cycle, thermomechanical, permeation, leak, and burst testing of full-scale hydrogen systems
- Thermal compression reduces station cost by eliminating expensive, maintenance prone compressors
- LLNL is leveraging high-performance computing, synthesis, and characterization capabilities in the HyMARC consortium to provide tools and understanding for developing future all-solid-state hydrogen storage solutions
- LLNL is leading computational research supporting advancement of solar-to-hydrogen conversion technology as a part of multi-lab multi-disciplinary R&D program (winner of 2014 DOE Hydrogen and Fuel Cells R&D Award)
- Modeling efforts have aided steady progress of experimental partners toward DOE performance goal of 25% solar-to-hydrogen energy conversion efficiency (FY16 record: 15 % by NREL)