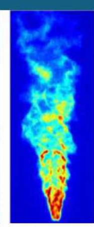
SAND2019-12068PE

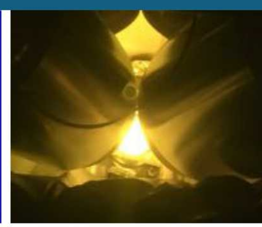
Sandia National Laboratories

# Hydrogen and Fuel Cells ($H_2FC$) Program

*Enabling Hydrogen Technologies with Science and Engineering*

*CSU – East Bay*
*Oct. 11, 2019*




PRESENTED BY

Jon Zimmerman and Mark Allendorf

jzimmer@sandia.gov


U.S. DEPARTMENT OF ENERGY NNSA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SAND2019-6463 PE

# Sandia Brings Value through Research in Materials and Safety

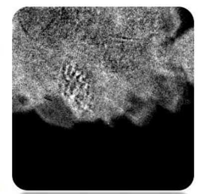
Sandia provides deep, quantitative understanding and a scientific basis for…

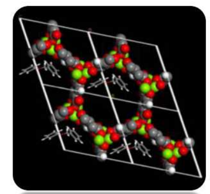
**Materials** – for hydrogen production, storage and utilization

**Safety** – risk analysis and the creation of risk-informed standards

## Hydrogen Storage Materials and Solutions

Discovering the behavior and performance of solid storage materials

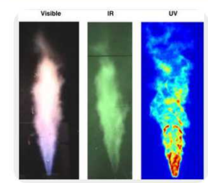




## Hydrogen Production from Renewables

Advanced water-splitting materials and technologies for large-scale $H_2$ production

## Hydrogen Fueling Infrastructure




$H_2$ release behavior and risk assessment to define the safety envelope for storage & delivery

## Hydrogen-Materials Compatibility

Low-cost, hydrogen-compatible materials and the science basis for their qualification

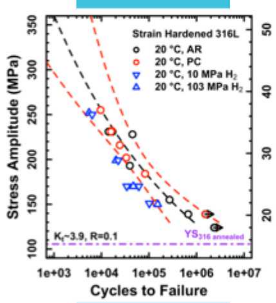
## Technologies for Non-Vehicle Applications

Marine and rail applications

# Developing the Technical Basis for Safety, Codes & Standards (SCS)

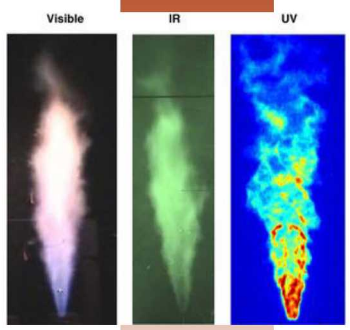
- Eliminate deployment barriers by informing codes and standards.

## Hydrogen-Materials Compatibility




*Understand material behavior*

## Hydrogen Behavior



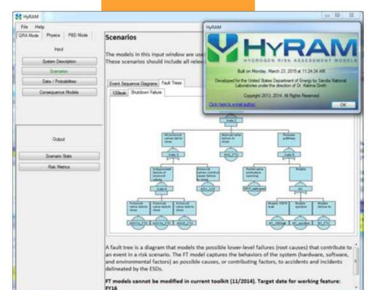

*Develop and validate scientific models*

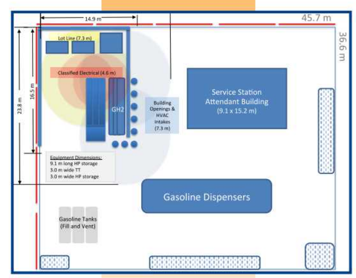
## Quantitative Risk Assessment

| Specific Component Type | Severity | Frequency | Units | Leak Size Description |
|---|---|---|---|---|
| Piping | | | | |
| Pipe Diameter (d) < 50 mm | Rupture | 1.00E-06 | Per Meter Year | 100% cross sectional area |
| d < 50 mm | Major | 5.00E-06 | Per Meter Year | 1" (25 mm) |
| 50 mm ≤ d < 149 mm | Rupture | 5.00E-07 | Per Meter Year | 100% cross sectional area |
| 50 mm ≤ d < 149 mm | Medium | 2.00E-06 | Per Meter Year | 1" (25 mm) |
| 150 mm ≤ d < 299 mm | Rupture | 2.00E-07 | Per Meter Year | 100% cross sectional area |
| 150 mm ≤ d < 299 mm | Major | 4.00E-07 | Per Meter Year | 1/3 of pipe diameter |
| 150 mm ≤ d < 299 mm | Minor | 7.00E-07 | Per Meter Year | 1" (25 mm) |
| 300 mm ≤ d < 499 mm | Rupture | 7.00E-08 | Per Meter Year | 100% cross sectional area |
| 300 mm ≤ d < 499 mm | Major | 2.00E-07 | Per Meter Year | 1/3 of pipe diameter |
| 300 mm ≤ d < 499 mm | Medium | 4.00E-07 | Per Meter Year | 2" (50 mm) |
| 300 mm ≤ d < 499 mm | Minor | 5.00E-07 | Per Meter Year | 1" (25 mm) |
| 500 mm ≤ d < 1000 mm | Rupture | 2.00E-08 | Per Meter Year | 100% cross sectional area |
| 500 mm ≤ d < 1000 mm | Major | 1.00E-07 | Per Meter Year | 1/3 of pipe diameter |
| 500 mm ≤ d < 1000 mm | Minor | 2.00E-07 | Per Meter Year | 2" (50 mm) |
| 500 mm ≤ d < 1000 mm | Very Small | 4.00E-07 | Per Meter Year | 1" (25 mm) |

*Apply quantitative risk assessment techniques*

## Integration

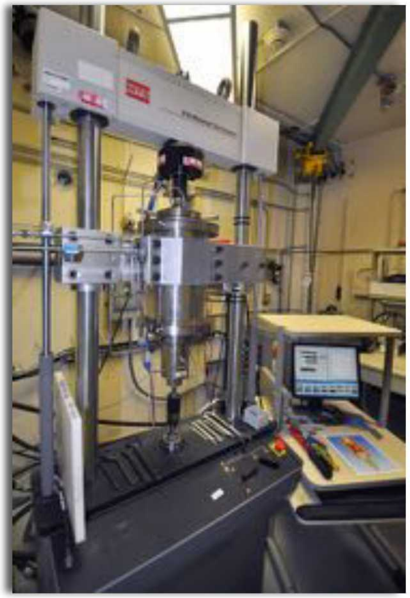


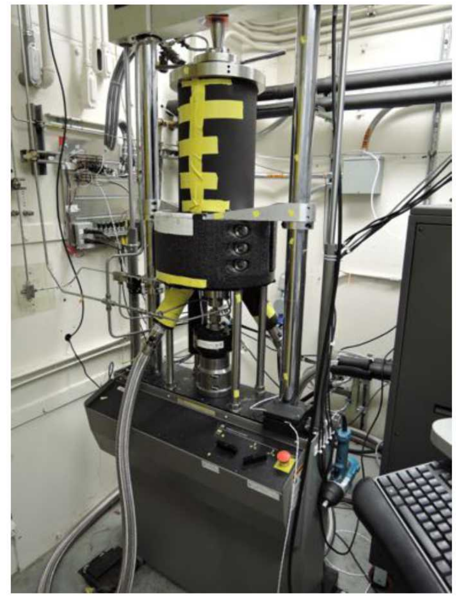




*Develop integrated methods and algorithms*

# Hydrogen Effects on Materials Laboratory

This lab houses specialized equipment for evaluating materials in high-pressure gaseous hydrogen.

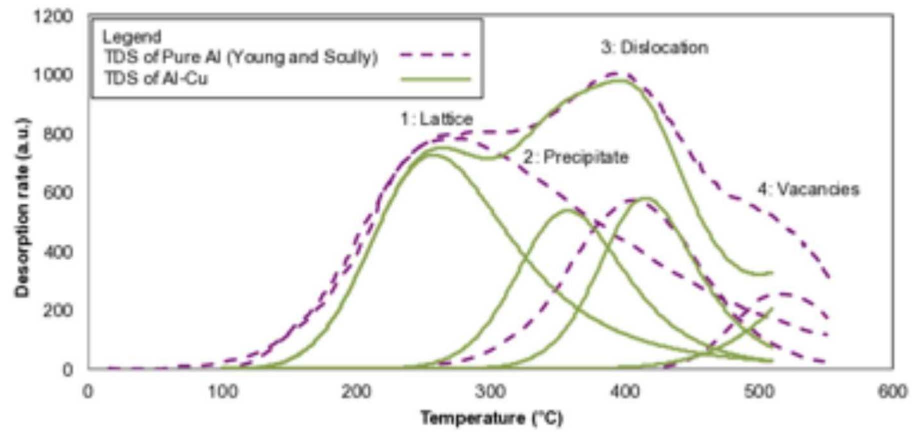




- **Fracture, fatigue and tensile testing** in high-pressure gaseous hydrogen at controlled temperature
- **Constant-displacement crack growth** testing in gas
- **Thermal pre-charging** to produce specific $H_2$ content
- **Pressure cycling** of metals and non-metals in controlled pressure and temperature

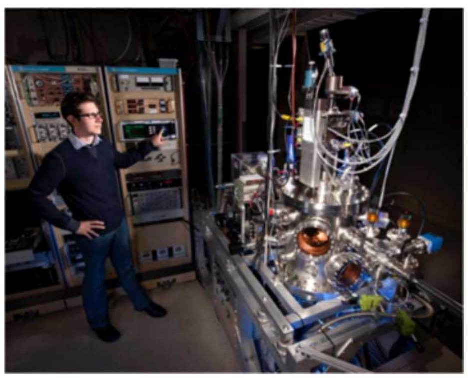
**B.P. Somerday *et al*, *International Journal of Hydrogen Energy* (2017)**

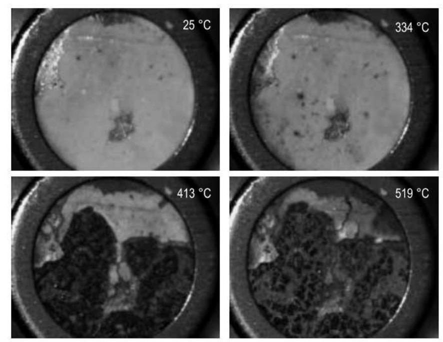
**Hydrogen Transport and Trapping Laboratory**: measuring diffusion of hydrogen in and through materials

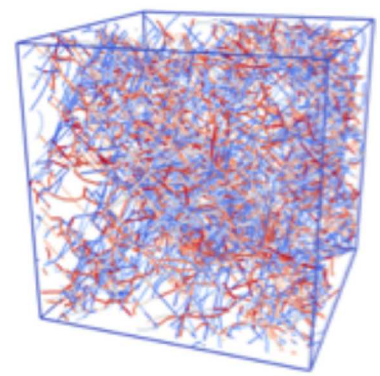



**Hydrogen Surface-Interactions Laboratory**:

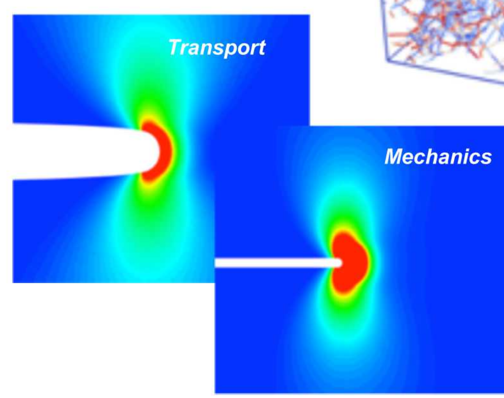
measuring adsorption and desorption of hydrogen at a material's surface





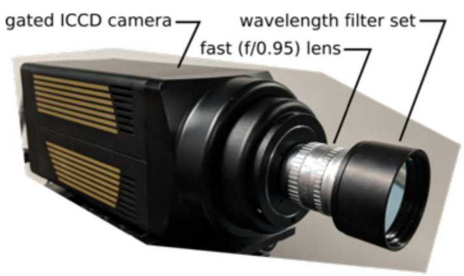



**Computational Materials Science**: models for studying the mechanisms of hydrogen-assisted behavior, and the evolution of microstructural features (e.g. dislocations, grain boundaries).

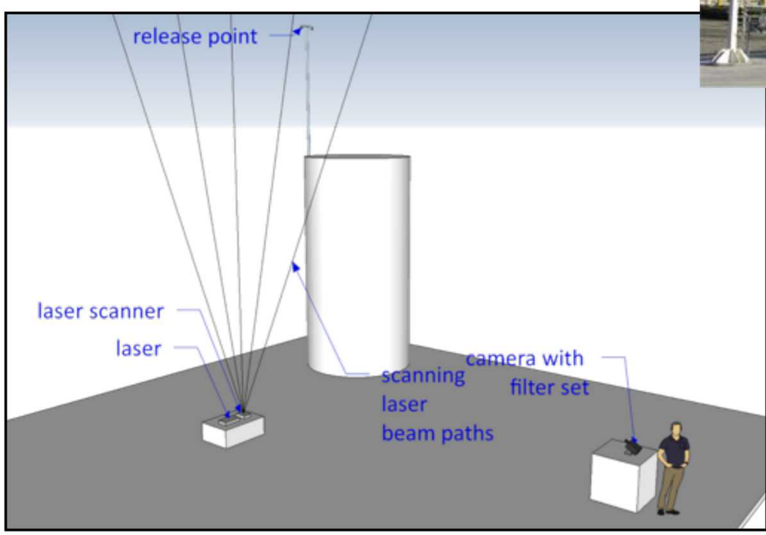


# Diagnostics for Large-Scale Releases

- Standards committees needs validation of our physical models on large-scale gaseous and liquid hydrogen releases.
- Developing diagnostic to measure quantitative characteristics (i.e. temperature, velocity, concentration) of large-scale releases under realistic environmental conditions (e.g. wind).








# Tunnel Safety for Urban Use of Fuel Cell Electric Vehicles

- Success of FCEVs requires assessing whether hydrogen vehicle use in tunnels presents challenges that differ from other fuels.


Fire Technology
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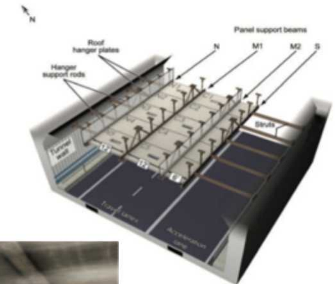
https://doi.org/10.1007/s10694-019-00910-z

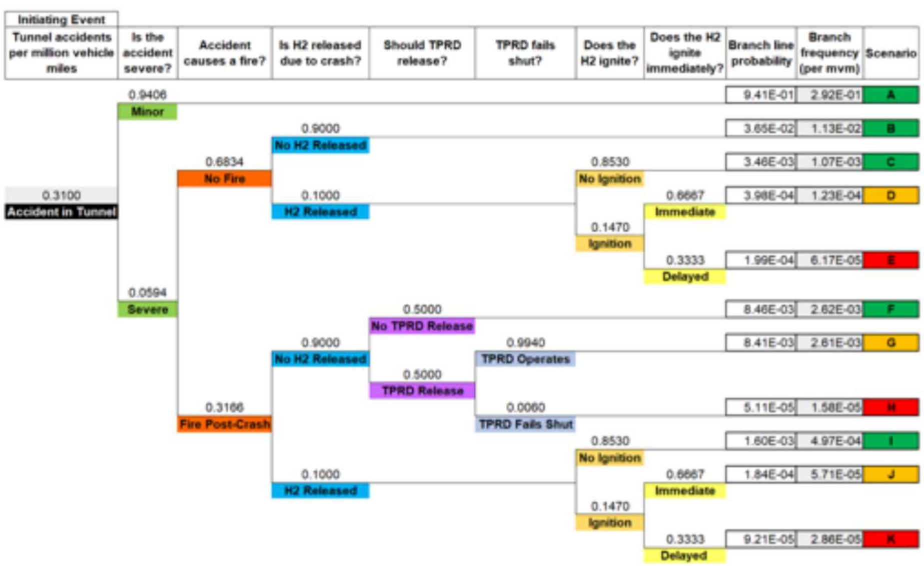
**Risk Assessment of Hydrogen Fuel Cell Electric Vehicles in Tunnels**

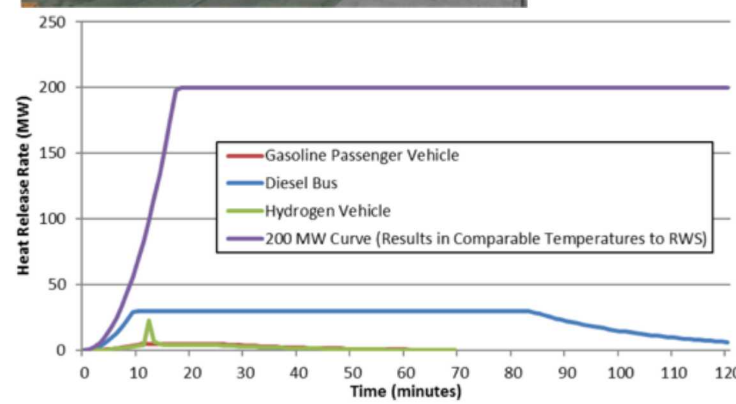
*Brian D. Ehrhart, Dusty M. Brooks, Alice B. Muna and Chris B. LaFleur*, Sandia National Laboratories, Albuquerque, NM 87*
*USA*

**Received:** 23 August 2018/**Accepted:** 14 Se




**Scenario of concern for Boston AHJ: overturned vehicle with TPRD pointed toward tunnel ceiling**



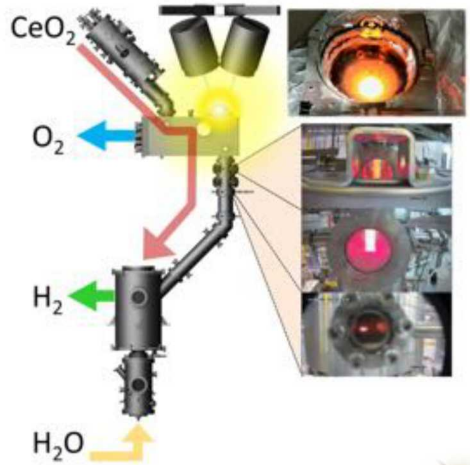



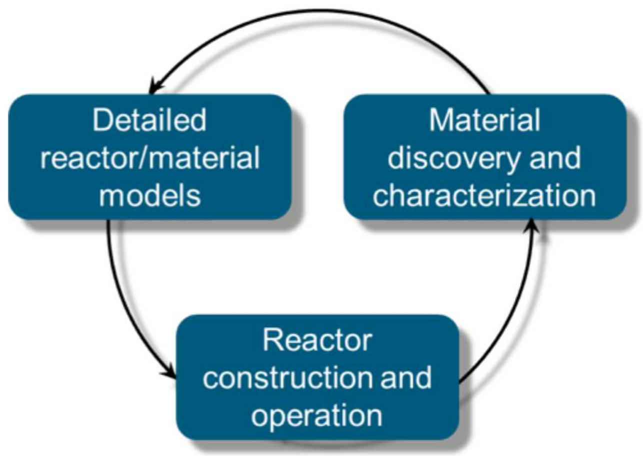

Ehrhart, Brian D., Muna, Alice B., LaFleur, Chris, "Risk Assessment of Hydrogen Fuel Cell Vehicles in Tunnels," Accepted by *Fire Technology*.

**FCEV releases less energy than a typical Heavy Goods Vehicle fire**

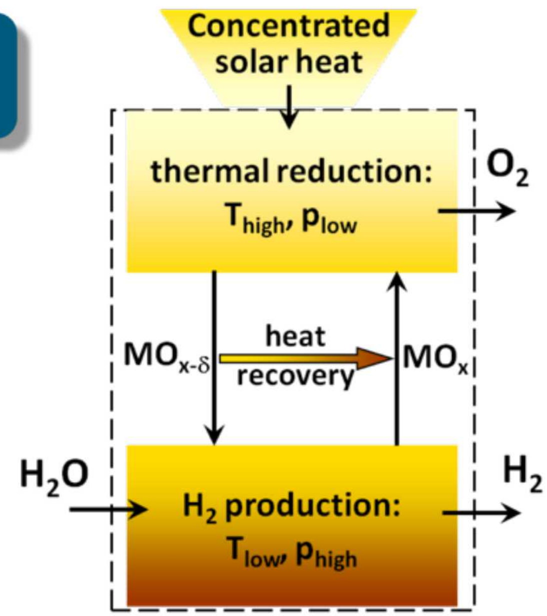
# Solar Thermo-Chemical Hydrogen Production (STCH)

- Clean and sustainable hydrogen production at large-scale is needed to realize emissions reductions over steam methane reforming (SMR).
- Solar heat can thermo-chemically induce water-splitting in some materials.




**CPR[2] technology produced 2 liters of hydrogen on simulated sun.**




Two-step metal oxide cycle

# Early-Market Demonstration of Hydrogen Fuel Cell Technology

## Hydrogen Fuel Cell Mobile Light Tower


## Hydrogen Fuel Cell Generator for Maritime/Ports

YOUNG BROTHERS

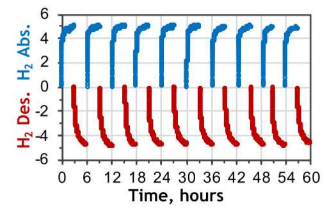
## Zero Emission Maritime Vessels

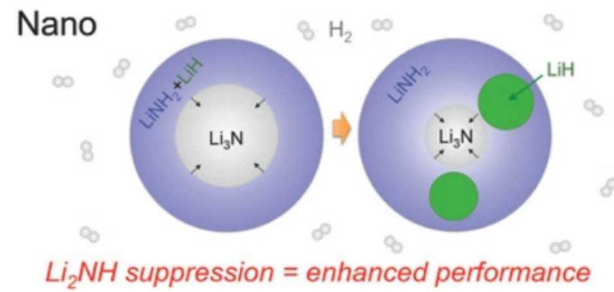

# Advances in Materials for Hydrogen Fuel Cell Technologies

- Hydrogen **production**, **storage** and **utilization** rely on low-cost, high-performing materials.

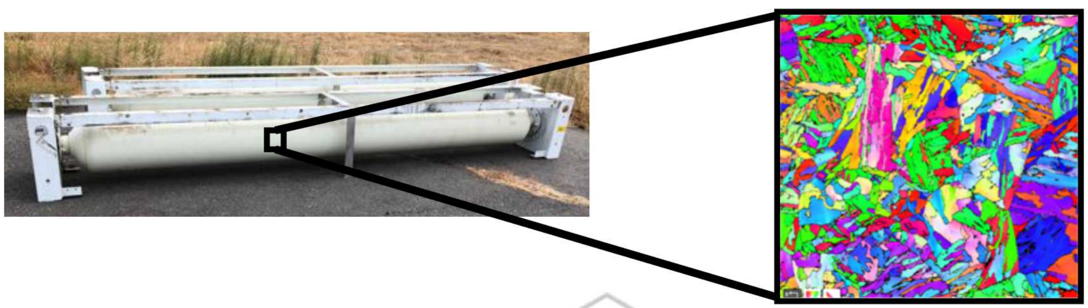
- **Nano-structuring for hydrogen storage materials**

HyMARC
Hydrogen Materials Advanced Research Consortium



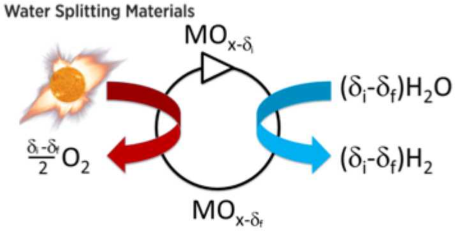

- **Alternative microstructures improve fracture toughness of storage tank steels**

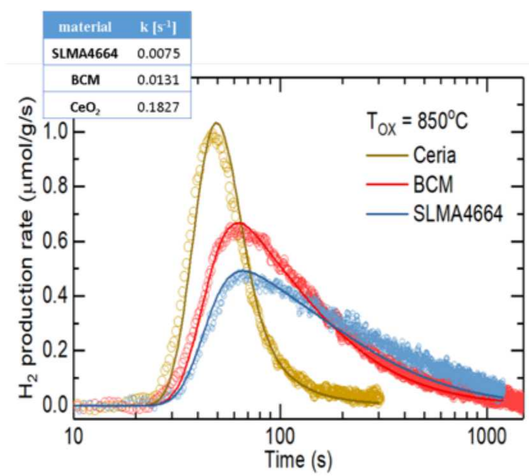


H-Mat
Hydrogen Materials Compatibility Consortium

- **New materials for solar thermo-chemical hydrogen production**

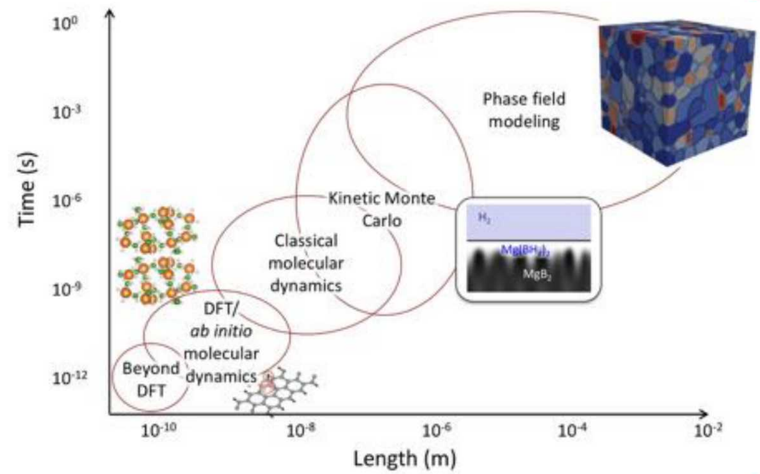
HydroGEN
Advanced Water Splitting Materials



# HyMARC objective: accelerate discovery of breakthrough storage materials by providing capabilities and foundational understanding

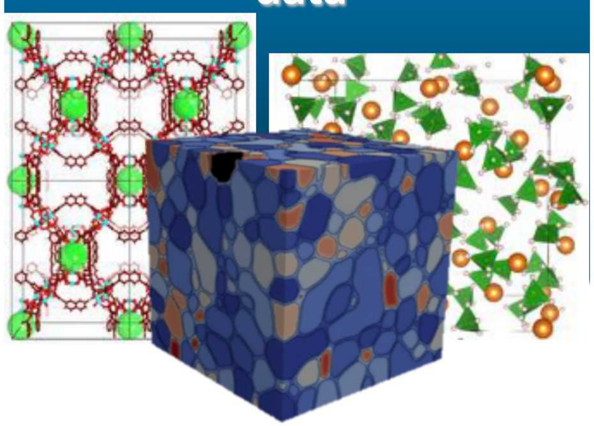
**Foundational understanding** of phenomena governing thermodynamics and kinetics limiting the development of solid-state hydrogen storage materials



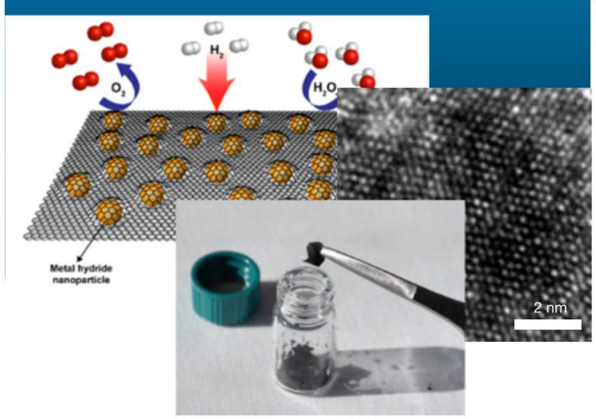

HyMARC will deliver **community tools and capabilities:**

- **Computational models and databases** for high-throughput materials screening
- **New characterization tools and methods** (surface, bulk, soft X-ray, synchrotron)
- **Tailorable synthetic platforms** for probing nanoscale phenomena

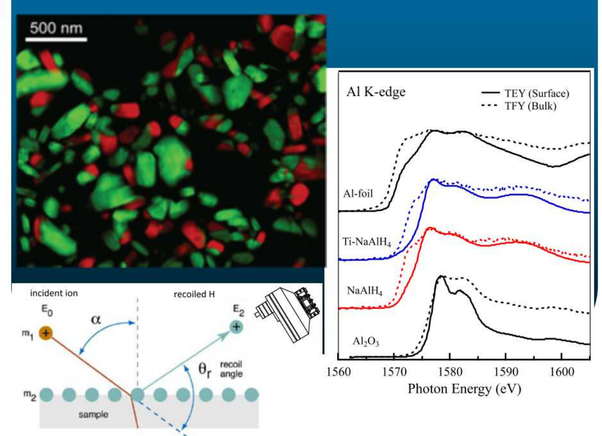
**Theory, simulation, & data**



**Controlled synthesis**



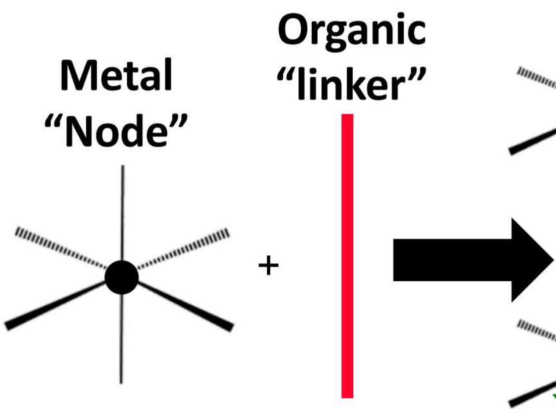

***In situ* characterization**

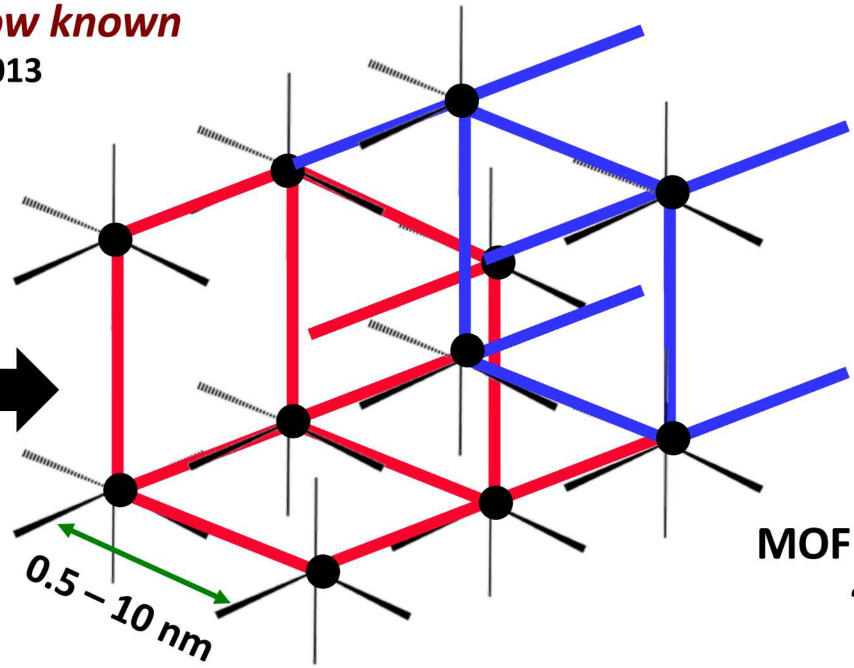


# Metal-Organic Frameworks (MOFs) are among the most promising hydrogen sorbents

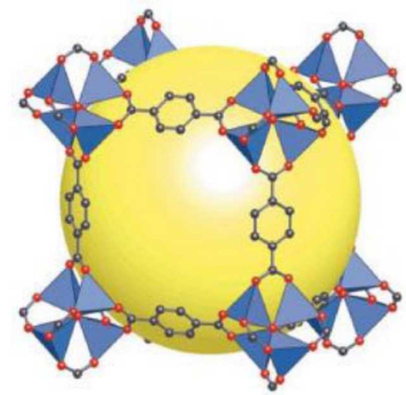
***Thousands of MOFs are now known***

**e.g. see Furukawa et al. *Science* 2013**

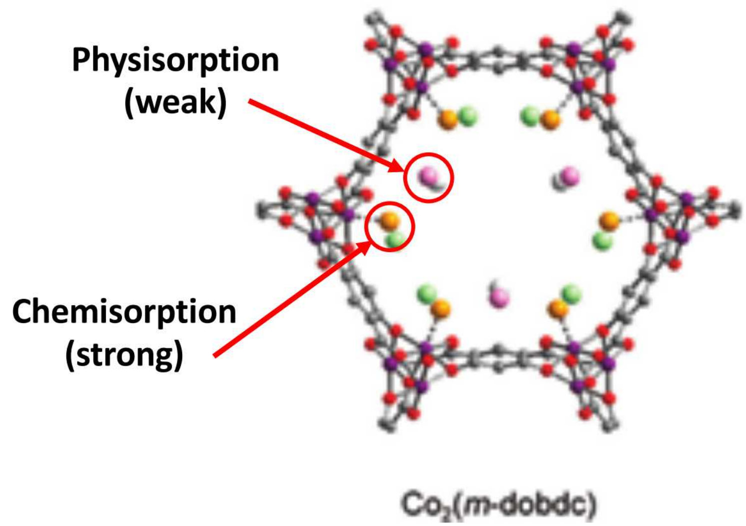


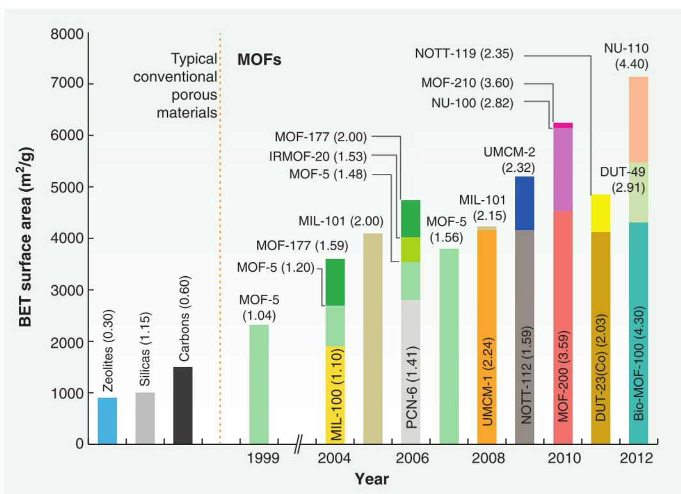

**MOF-5**



**MOF $H_2$ binding energies ~ 2 – 33 kJ/mol**




## Record surface areas



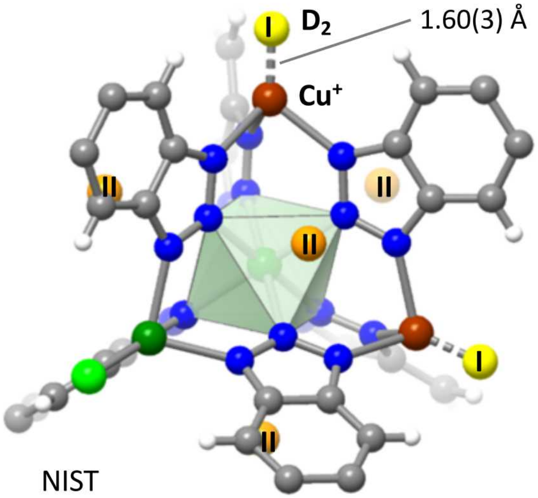

O.M. Yaghi et al. *Science* **341** (2013), 974

Allendorf, M. D. Hulvey, Z., T. Gennett et al.
*Energy & Environ. Sci.* **11** (2018), 2784. DOI: 10.1039/C8EE01085D

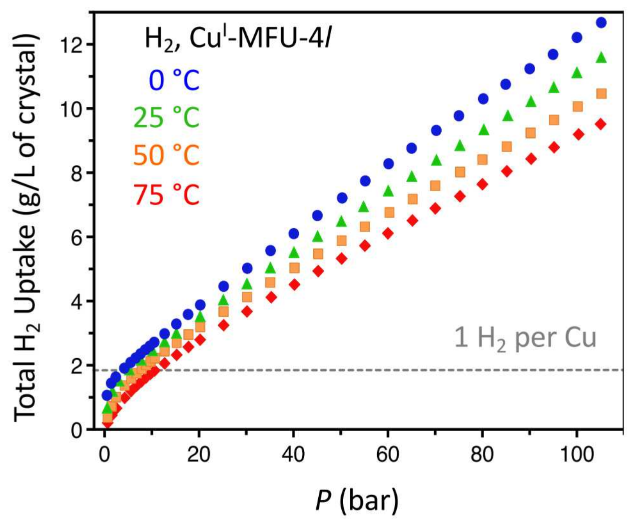
# Recent HyMARC research indicates H2 binding energies can be increased in MOFs

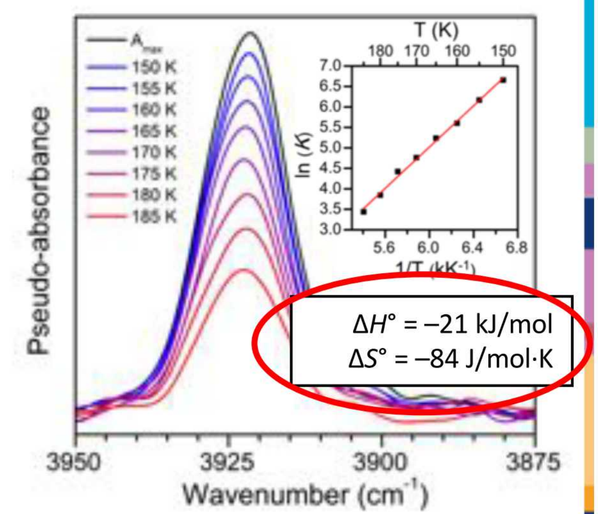
## *Copper and Vanadium MOFs have heats of adsorption 21 – 33 kJ mol$^{-1}$*

**Research of J. R. Long and coworkers**




NIST



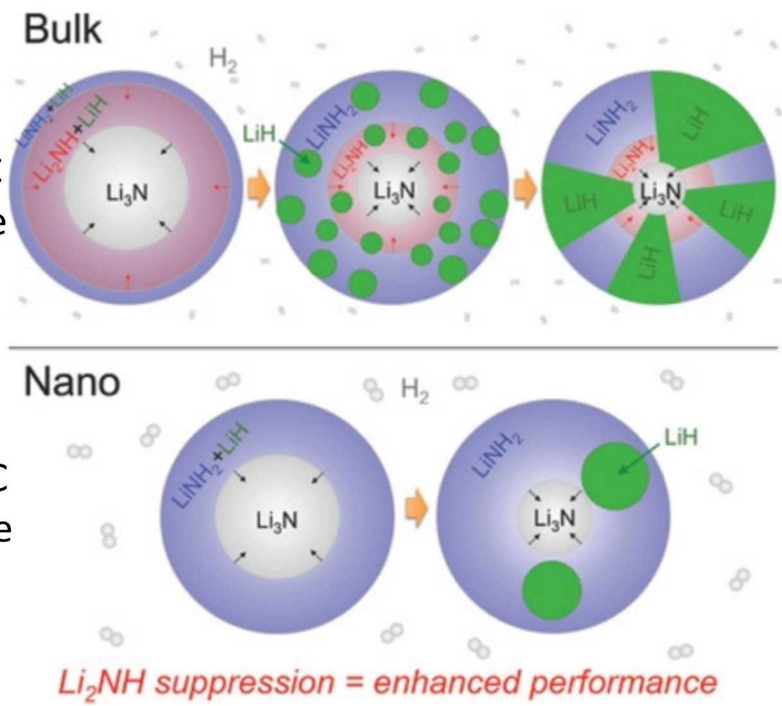




- ***In situ* powder neutron diffraction:** Extremely short Cu–$D_2$ distance observed in $Cu^I$-MFU-4*l* by neutron powder diffraction. Corroborates strong binding enthalpy and large red-shift of u(H–H) observed from DRIFTS.
- **High-P adsorption:** Open $Cu^+$ sites saturate at relatively low pressures. Volumetric usable capacity for $Cu^I$-MFU-4*l* surpasses $Ni_2$(*m*-dobdc) at 75 °C.
- **DRIFTS in $V_2Cl_{2.8}$(btdd):** VTIR confirms high enthalpy of adsorption. Enthalpy–entropy relation distinct from $M_2$(dobdc) family.

# Nanoscale metal hydrides have faster H2 uptake and release

430 °C release

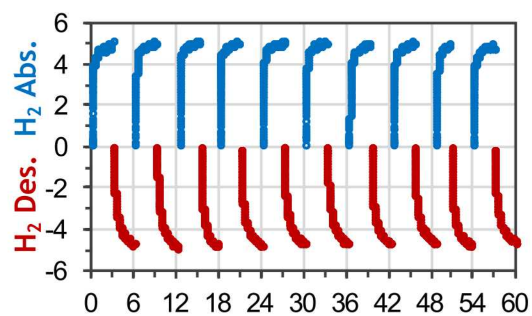
250 °C release




B. C. Wood *Adv. Mater. Interfaces* (2017)
https://doi.org/10.1002/admi.201600803

*Metal Hydride Finite Element model reveals non-intuitive tradeoffs and benefits of using nanoscale metal hydrides in an operational $H_2$ storage tank*

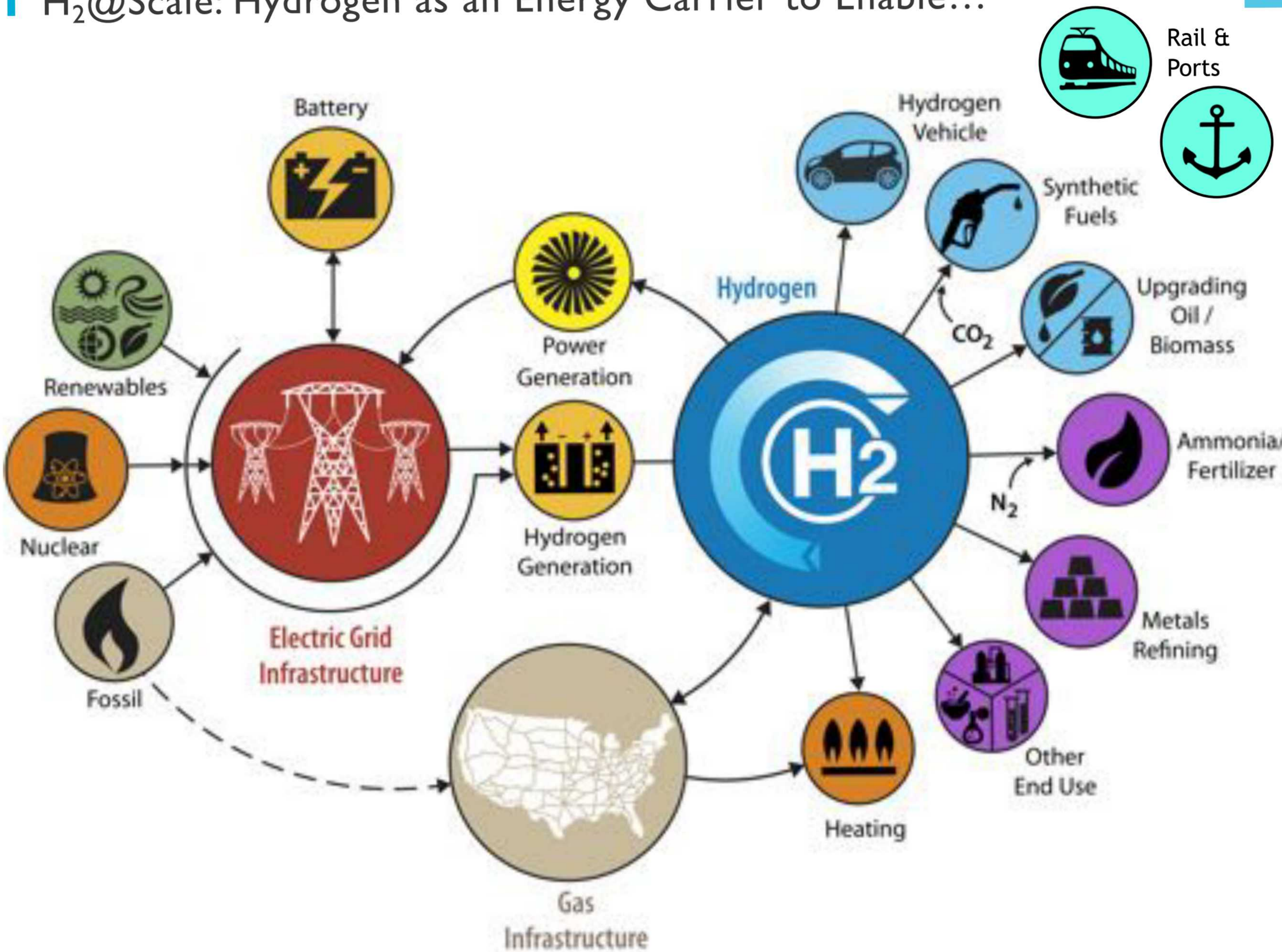
| Design Parameters | bulk-$Li_3N$ | KH-6nm-$Li_3N$ |
|---|---|---|
| Reversible capacity. wt% | 8.2 | 5.4 |
| Thermal cond., W $m^{-1}$ $K^{-1}$ | 1.0 | 9.6 |
| Density of hydride bed, kg $m^{-3}$ | 710 | 760 |
| Total system mass, kg | 312 | 252 |
| Total hydride mass, kg | 112 | 116 |
| Tank outer diameter, m | 0.46 | 0.45 |
| Tank length, m | 2.21 | 2.19 |
| System volume, $m^3$ | 0.256 | 0.227 |
| % 2025 Gravimetric Target | 33 | 40 |
| % 2025 Volumetric Target | 55 | 62 |




MHFE-SAH tank design

# Customers and Partners

# $H_2$@Scale: Hydrogen as an Energy Carrier to Enable…



# BACKUP SLIDES

# Hydrogen Fueling Infrastructure Research and Station Technology (H2FIRST)

- Goal: Address challenges/obstacles to hydrogen fueling station deployment.


NREL Sandia National Laboratories
H2FIRST H2USA

H2FIRST Reference Station Design Task

Project Deliverable 2-2

Joseph Pratt
*Sandia National Laboratories*

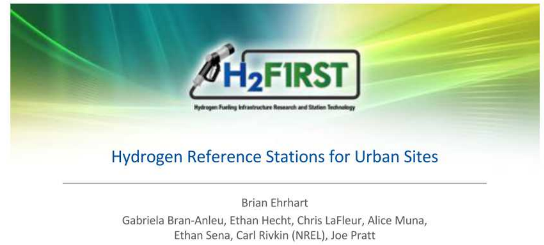
Danny Terlip, Chris Ainscough, Jennifer Kurtz
*National Renewable Energy Laboratory*

Amgad Elgowainy
*Argonne National Laboratory*


NREL Sandia National Laboratories
H2FIRST H2USA

Comparison of conventional vs. modular hydrogen refueling stations, and on-site production vs. delivery

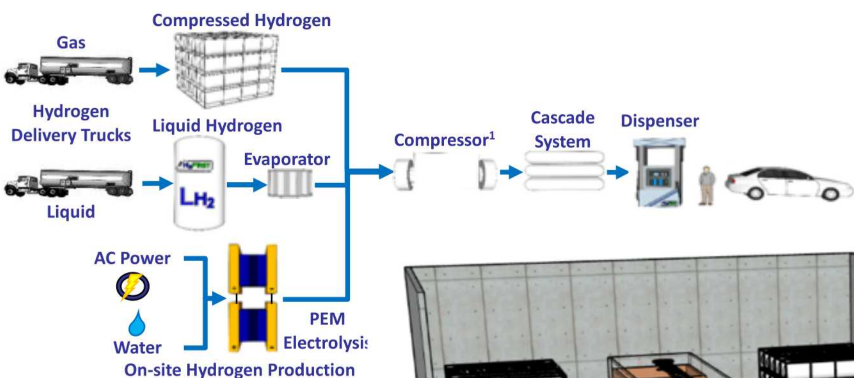
Ethan S. Hecht, Joseph Pratt
Sandia National Laboratories

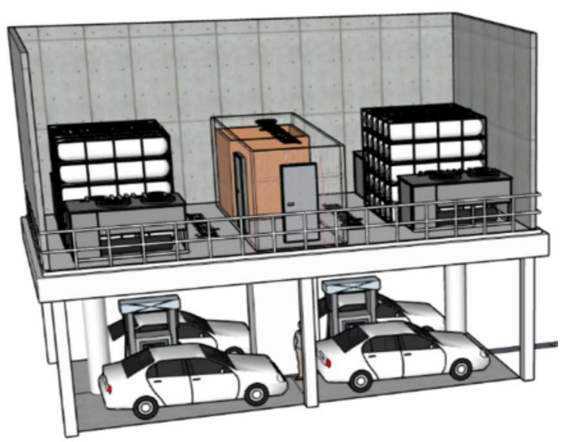

H2FIRST

Hydrogen Reference Stations for Urban Sites

Brian Ehrhart
Gabriela Bran-Anleu, Ethan Hecht, Chris LaFleur, Alice Muna, Ethan Sena, Carl Rivkin (NREL), Joe Pratt

Building off of previous reference design projects to increase station capacity, reduce footprint and improve station details



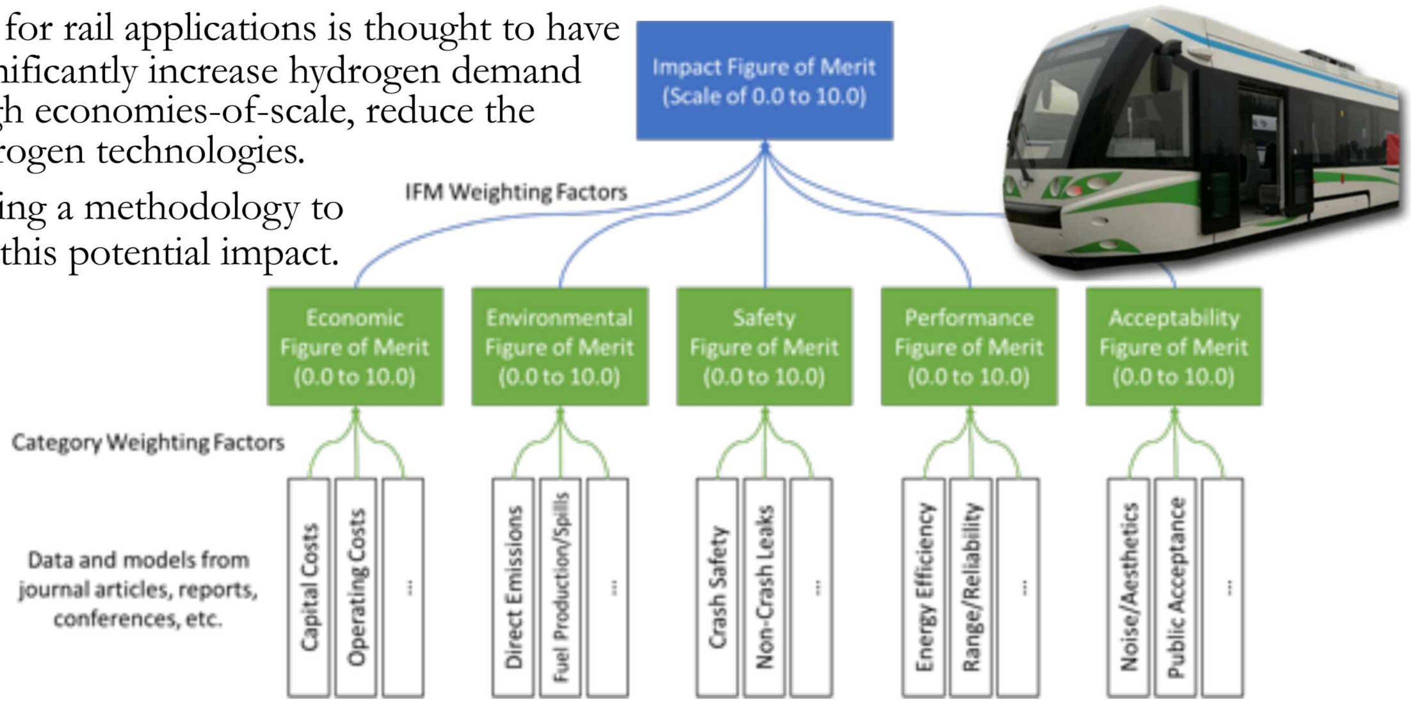



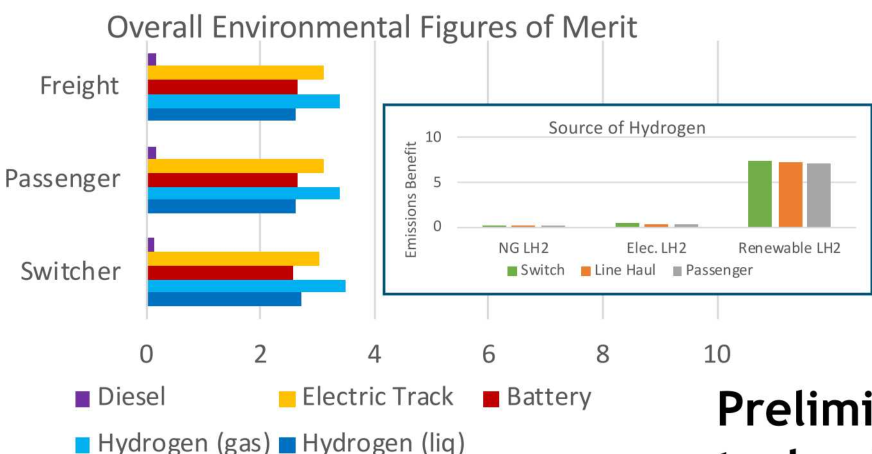
| | Total Lot Area (ft$^2$) | Reduction from Base Case |
|---|---|---|
| Base Case Gas | 17,640 | -- |
| New NFPA Separation Distances | 16,240 | 7.9% |
| New Delivery Single Truck | 14,500 | 17.8% |
| New Delivery Double Truck | 15,875 | 10.0% |
| Gasoline Co-Location | 21,000 | -19.0% (Increase) |
| Underground Direct-Bury | 15,400 | 12.7% |
| Underground Vault | 13,720 | 22.2% |
| Rooftop Storage | 16,000 | 9.3 % |

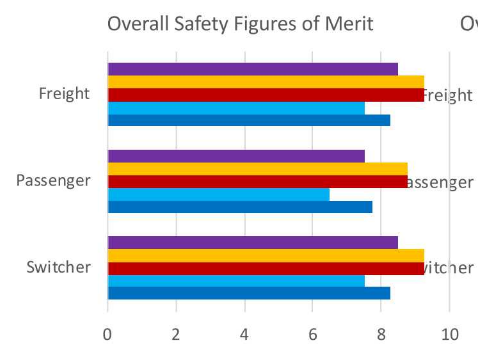
| | Total Lot Area (ft$^2$) | Reduction from Base Case |
|---|---|---|
| Base Case Liquid | 21,250 | -- |
| New NFPA Separation Distances | 18,252 | 14.1% |
| New Liquid Delivery | 17,400 | 18.1% |
| Gasoline Co-Location | 22,040 | -3.7% (Increase) |
| Underground Direct-Bury | 15,515 | 27.0% |
| Rooftop Storage | 19,840 | 6.63 % |

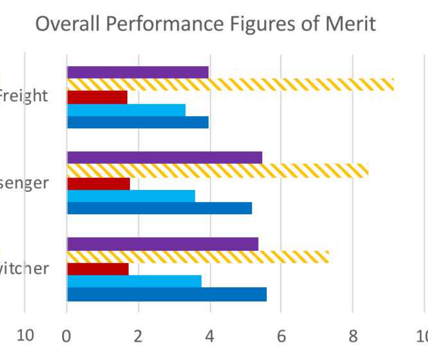
# Assessing the Impact of Hydrogen for Rail ($H_2$@Rail)

- Use of hydrogen for rail applications is thought to have the potential to significantly increase hydrogen demand and thereby, through economies-of-scale, reduce the overall cost of hydrogen technologies.
- Sandia is developing a methodology to evaluate and verify this potential impact.


**Preliminary results show trade-offs between all technologies → *More refinement needed***

# H-Mat: Science-Based Advancement of Materials for Hydrogen Technologies

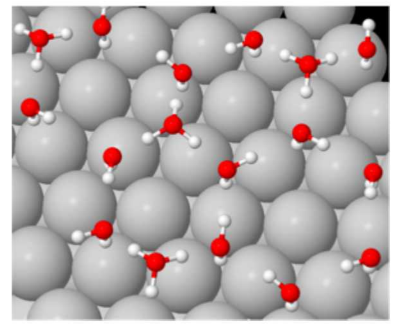
- Elucidate the mechanisms of hydrogen-materials interactions to inform **science-based strategies to design the microstructure** of metals with improved resistance to hydrogen degradation

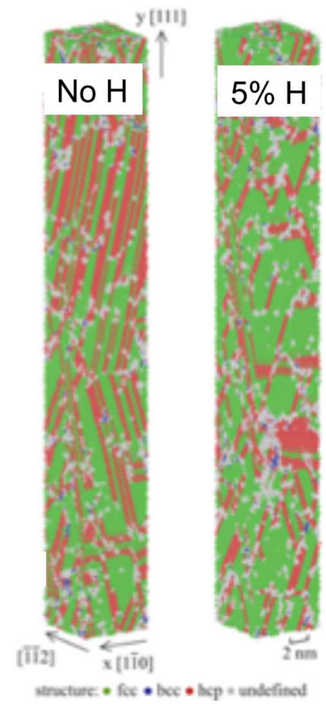
H-Mat Hydrogen Materials Compatibility Consortium

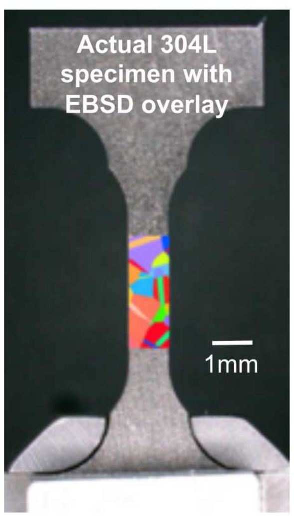
Sandia National Laboratories · Pacific Northwest National Laboratory · Argonne National Laboratory · Oak Ridge National Laboratory · SRNL

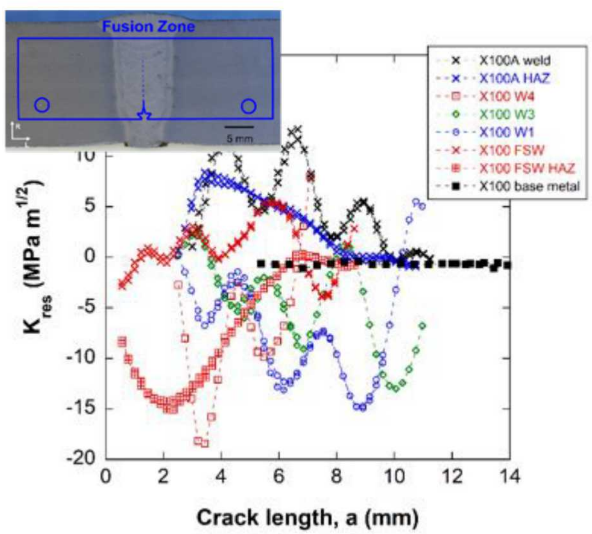
Tasks include:

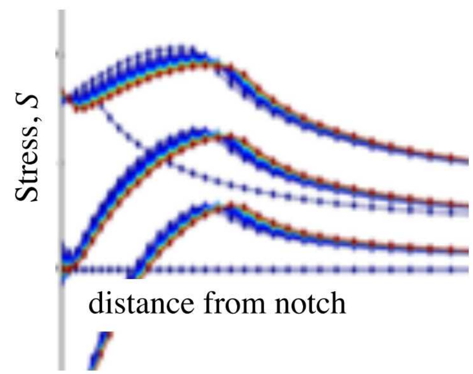
- High-strength ferritic steel microstructures
- High-strength aluminum alloys
- Transferability of damage and crack nucleation
- Microstructure of austenitic stainless steels
- Materials for cryogenic hydrogen service
- Mechanisms of polymer degradation
- Multiscale modeling of polymer materials
- Hydrogen-resistant polymeric formulations





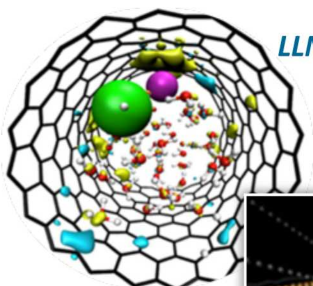




https://www.energy.gov/eere/fuelcells/h-mat-hydrogen-materials-consortium

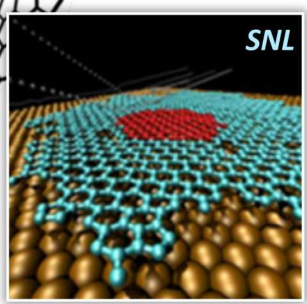
# HydroGEN: Advanced Materials for Water-Splitting for Low-Cost $H_2$

➢ HydroGEN combines more than 80 unique, word-class capabilities (nodes) to foster cross-cutting innovation in materials to advance all emerging water-splitting pathways for hydrogen production.

***Materials Theory/Computation***

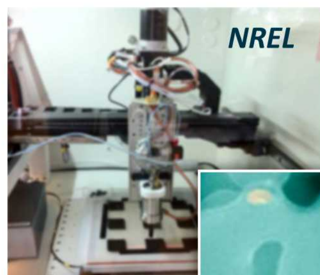



Bulk & interfacial models of aqueous electrolytes

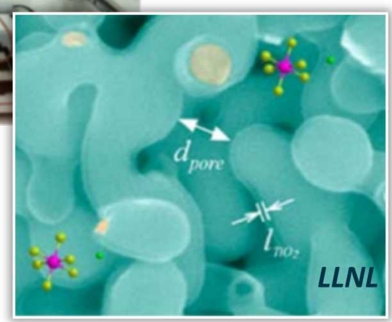



LAMMPS classic molecular dynamics modeling relevant to $H_2O$ splitting

***Advanced Materials Synthesis***

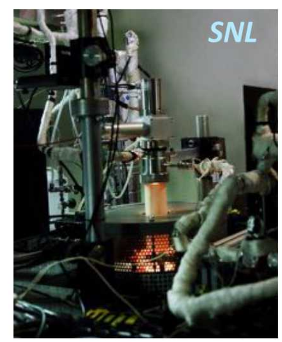



High-throughput spray pyrolysis system for electrode fabrication




Conformal ultrathin $TiO_2$ ALD coating on bulk nanoporous gold

***Characterization & Analytics***



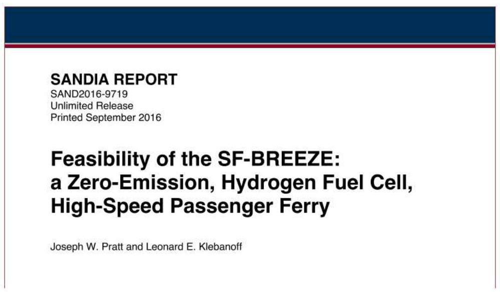

Stagnation flow reactor to evaluate kinetics of redox material at high-T


TAP reactor for extracting quantitative kinetic data

https://www.h2awsm.org/

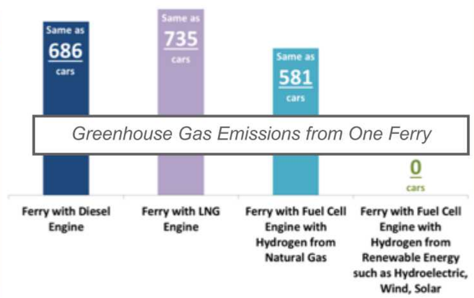
# Feasibility of Hydrogen Fuel Cell-Powered Maritime Vessels

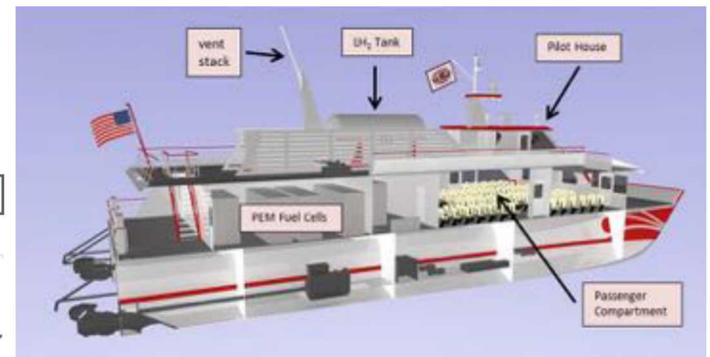
- Are hydrogen powered marine vessels feasible considering technical, economic and regulatory factors?
- SF-BREEZE high-speed passenger ferry
  - Catamaran design has similar capacity to existing ferry service.
  - Analysis shows modest emissions reduction with SMR-produced hydrogen , zero emission with renewable hydrogen.


**SANDIA REPORT**
SAND2016-9719
Unlimited Release
Printed September 2016

**Feasibility of the SF-BREEZE: a Zero-Emission, Hydrogen Fuel Cell, High-Speed Passenger Ferry**

Joseph W. Pratt and Leonard E. Klebanoff




- Zero-V coastal research vessel
  - Feasibility was found for a vessel able to perform 14 Scripps science missions with a 2,400 nautical mile range.