HyMARC: Addressing Key Challenges to Hydrogen Storage in Advanced Materials Through a Multi-Lab Collaboration

HyMARC
Hydrogen Materials Advanced Research Consortium

Enabling twice the energy density for onboard H_2 storage

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Tom Gennett, National Renewable Energy Laboratory

NREL NATIONAL RENEWABLE ENERGY LABORATORY · Sandia National Laboratories · Lawrence Livermore National Laboratory · Berkeley Lab · Pacific Northwest NATIONAL LABORATORY · NIST · SLAC NATIONAL ACCELERATOR LABORATORY

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Project ID: ST127

SAND2019-3177 PE

Overview

Timeline

Phase 1: FY16 – FY18
Phase 2 FY19 – FY22

Barriers

General:

- **A. Cost, B. Weight and Volume, C. Efficiency, E. Refueling Time**

Reversible Solid-State Material:

- **M. Hydrogen Capacity and Reversibility**
- **N. Understanding of Hydrogen Physi- and Chemisorption**
- **O. Test Protocols and Evaluation Facilities**

Budget (Entire HyMARC Team)

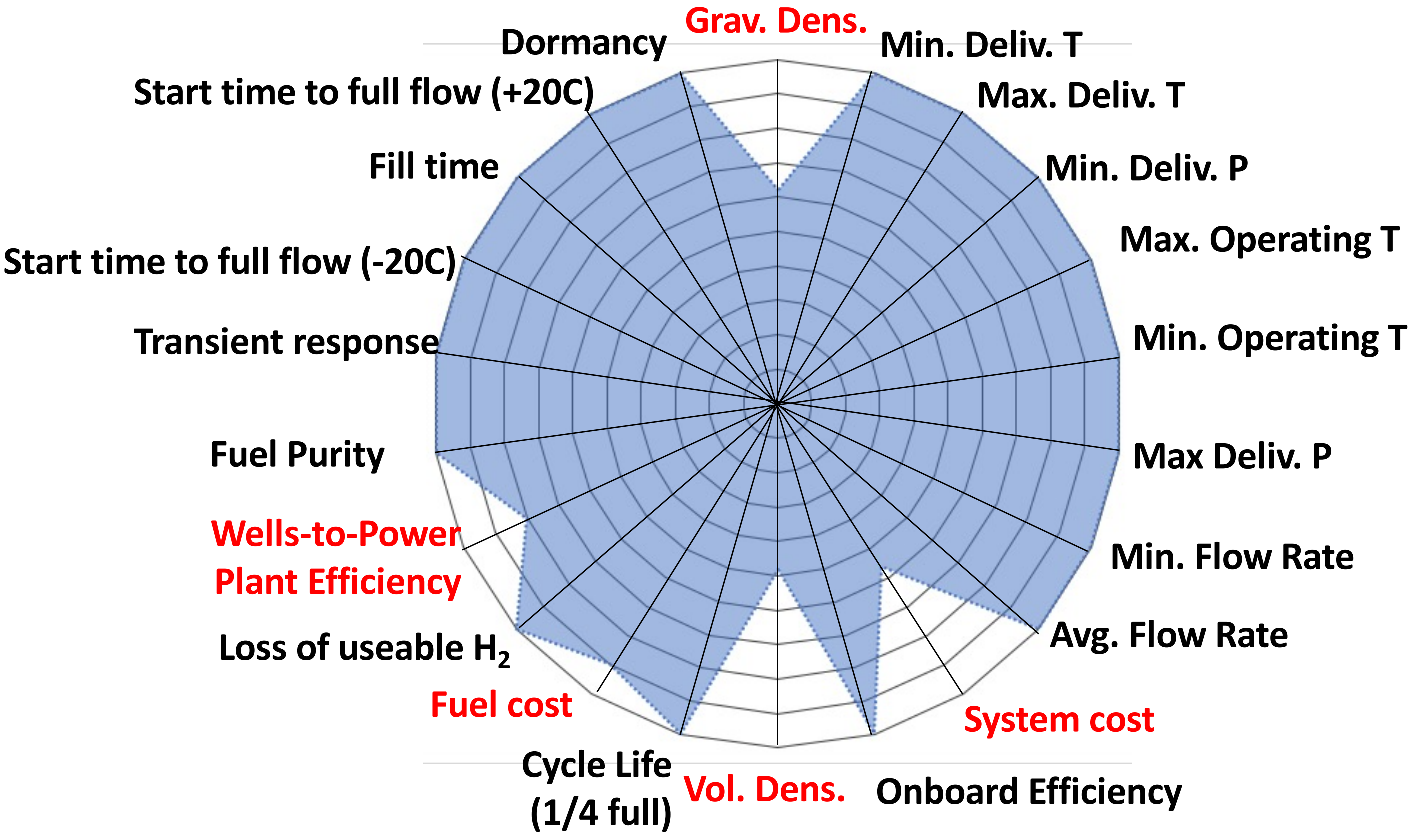
FY18 Phase 1 Funds:	**$3,820K**
FY18 DOE Funding for Phase 2:	**$5,501K**
FY19 DOE Funding (as of 3/31/19):	**$2,350K**
Total DOE Phase 2 Funds Received:	**$7,851K**

Partners

- **Sandia National Laboratories**
- **National Renewable Energy Laboratory**
- **Lawrence Livermore National Laboratory**
- **Lawrence Berkeley National Laboratory**
- **Pacific Northwest National Laboratory**
- **SLAC Accelerator Laboratory**
- **NIST Center for Neutron Research**

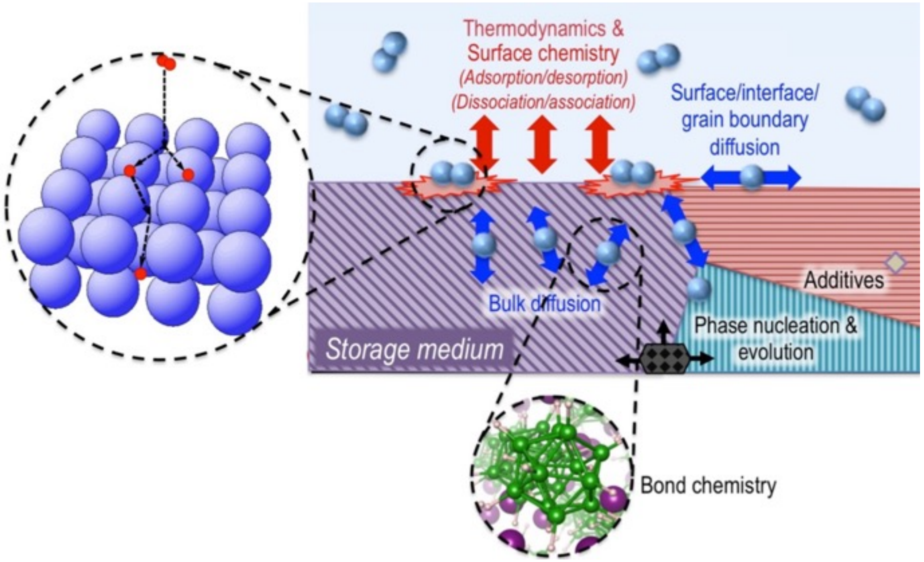
Relevance: Although fuel cell vehicles are now commercially available, compressed H_2 storage falls short of several DOE targets

700 Bar Compressed Gas (2015 record) vs. revised ultimate Targets

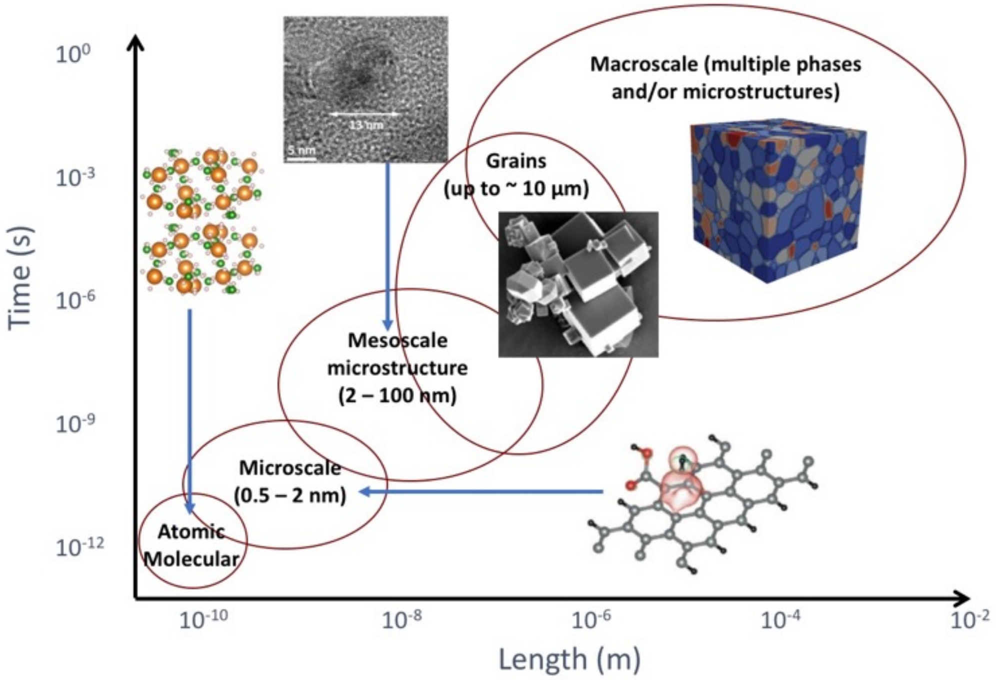


Relevance: poorly understood phenomena at length scales from < 1 nm to μm govern storage material behavior

Distinct chemical/physical processes affect the bulk properties of storage materials



Multiple length scales must be taken into account



"Design rules" are needed to guide materials discovery

Objective: HyMARC aims to accelerate materials discovery

Assemble small, agile teams comprising synthetic, characterization, and modeling expertise

Foundational knowledge gaps

- Model material systems
- Thermodynamic data
- Kinetic data
- Microstructural features

- **Structure-property relationships**
- **Rate-limiting steps**
- **What material features really matter?**

New core capabilities

- Computational models
- Characterization tools
- Novel material platforms

- **Probe and predict at all relevant length scales**
- **State-of-the-art tools for materials discovery**
- **Assist Seedling projects**

Evaluate new material concepts

- Assess potential
- Perform high-accuracy measurements

- **Define new research directions**
- **Provide guidance to DOE for funding investments**

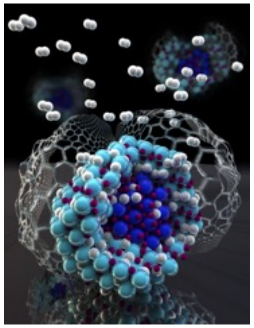
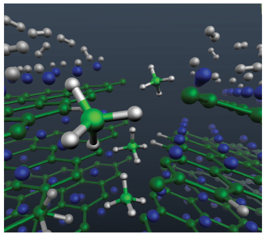
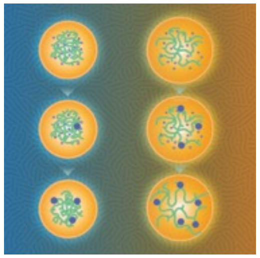
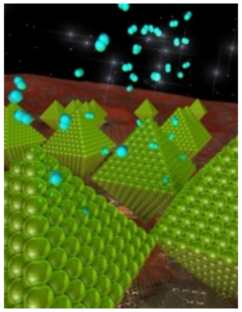
"Gold standard" measurements

- Variable T PCT
- Thermal conductivity
- Ultrahigh-pressure reactor

- **Validate claims, concepts, and theories**

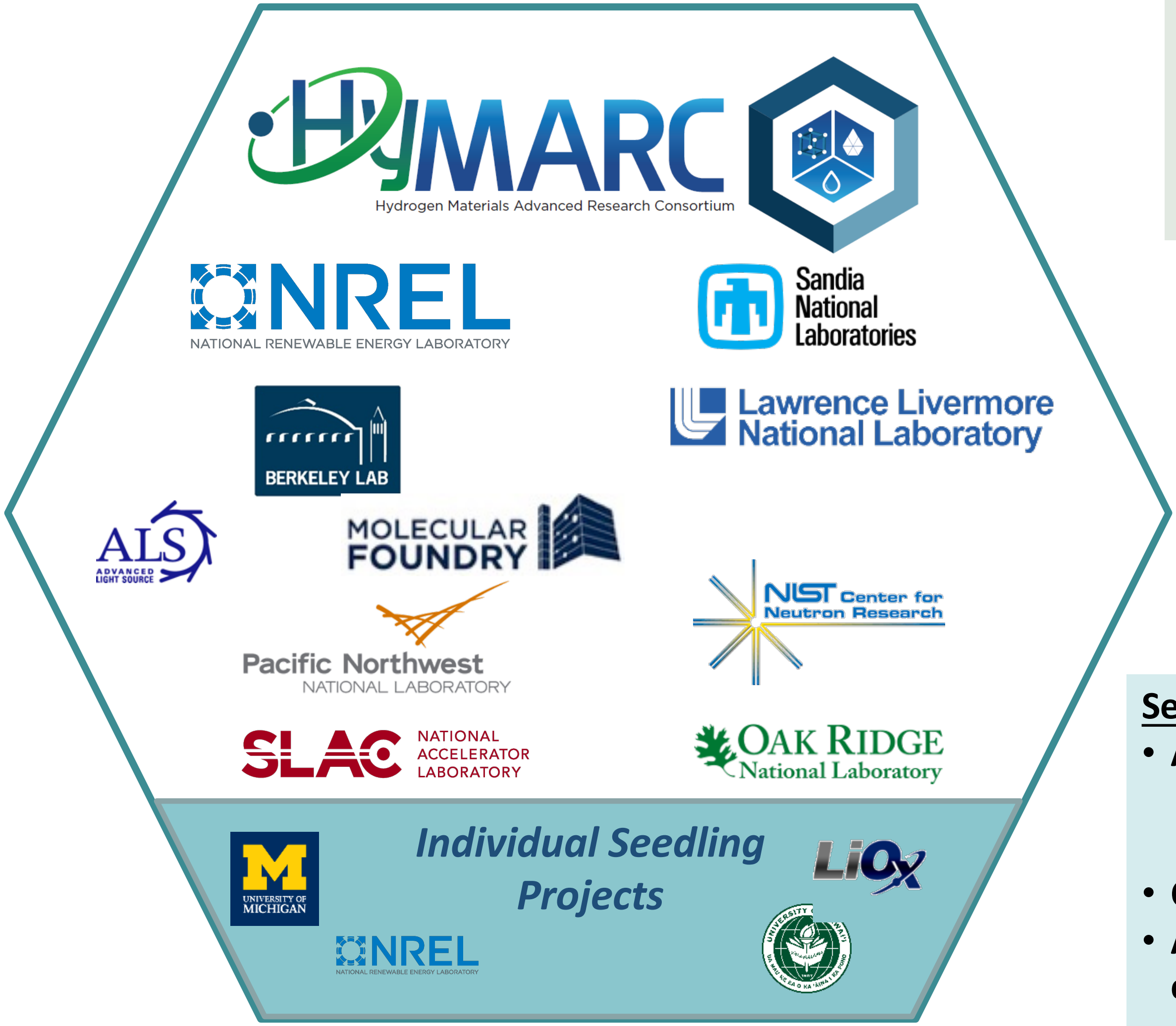
Accomplishments: HyMARC Phase 1 by the numbers

- **> 50 journal articles published**
  - Including articles in *Energy Env. Sci., Chem. Rev., Adv. Mater. Interfaces, Nat. Commun., Adv. Funct. Mater., Nano Lett., Chem. Mater.*
  - 4 articles on journal covers
  - 2 HOT articles
- **4 patents (3 issued, 1 applied)**
- **Numerous invited talks** (major international meetings, academic, gov't institutions)
- **6 Symposia and workshops organized** at major conferences
- **> 20 postdocs supported**
- **Global connectivity** through extensive network of collaborations

Approach/HyMARC-2 Energy Materials Network: enhanced, highly coordinated capabilities to accelerate materials discovery

Enabling twice the energy density for hydrogen storage



- **Foundational R&D**
- **Computational models**
- **Synthetic protocols**
- **Advanced characterization tools**
- **Validation of material performance**
- **Guidance to FOA projects**
- **Database development**

Seedling Projects

- **Applied material development**
  - Novel material concepts
  - High-risk, high-reward
- **Concept feasibility demonstration**
- **Advanced development of viable concepts**

Approach Phase 2: Build on Phase 1 discoveries using multi-lab Focus Area teams with interdisciplinary expertise

Tom Gennett (NREL)
Co-Director

Mark Allendorf (SNL)
Co-Director

Task 1
Sorbents
Gennett

Focus Areas

Task 2
Hydrides
Allendorf

Focus Areas

Task 3
Carriers
Autrey

Focus Areas

Task 4
Adv. Char.
Parrilla
(NREL validation)
Prendergast
(ALS, SLAC, MF)
Bowden
(PNNL NMR)
Brown
(NIST Neutron)
Toney
(SLAC, X-ray)

Focus Areas

Task 5
Seedling Support
Allendorf
Gennett

Task 6
Data Hub
Munch
(NREL)

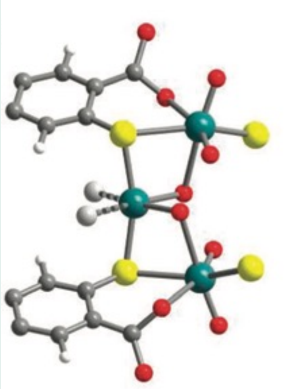
Task leads:
Coordinate work
Milestone accounting
Reporting

Focus Areas (new concept):
Multi—lab Research clusters
Defined topic
Dynamic, agile
Duration: as little as 1 year
Applied topics: Go/No-Go
Foundational topics: milestones

BES User Facility POCs

ALS
SLAC
NREL
NIST
EMSL
MOLECULAR FOUNDRY

Sorbents Phase 1 Accomplishments: moved the bar toward materials that meet DOE targets



Multiple molecular H_2 adsorption: First sorbent material with validated existence of two H_2 molecules adsorbed per metal center

→ Doubles the volumetric capacity of strong-binding sites

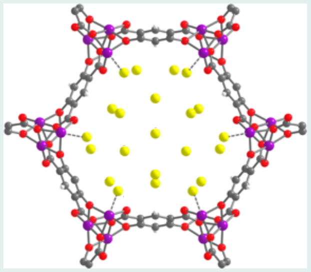
- *Chem. Commun.*, 2016, 8251

Highest validated volumetric capacity at room temperature to date:

Ni(m-dodbc): 11.0 g/L at 25 ˚C and 23.0 g/L for 5→100 bar pressure swing, −75 → 25 ˚C temperature swing

→ Demonstrates high capacity under realistic operating conditions

- *Chem. Mater.* 2018, **30**, 8179



H_2 binding energy in a MOF: within optimal range (15 – 25 kJ mole^{-1})

$V_2Cl_{2.8}$(btdd): Qst = 21 kJ mol^{-1}

→ Moving significantly closer to ambient-temperature storage

- see Slide 28 and ST130 for more information

New methodologies for validation

Improved accuracy of sorbent gas uptake measurements

- P.A. Parilla et al. *Appl. Phys. A* **122** (2016), 201
- K. E. Hurst et al. *Appl. Phys. A* **122:42** (2016) **DOI:** 10.1007/s00339-015-9537-x

Approach Sorbents Phase 2: building on Phase 1 discoveries

Key issues being addressed in Phase 2

- Need thermodynamics under practical conditions
- Crystallite size/shape/packing must be enhanced to improve capacity
- Can we tailor isotherms to increase capacity (5 – 100 bar swing)?
- Can volumetric density of strong-binding sites be increased?

Strategies based on Phase 1 results

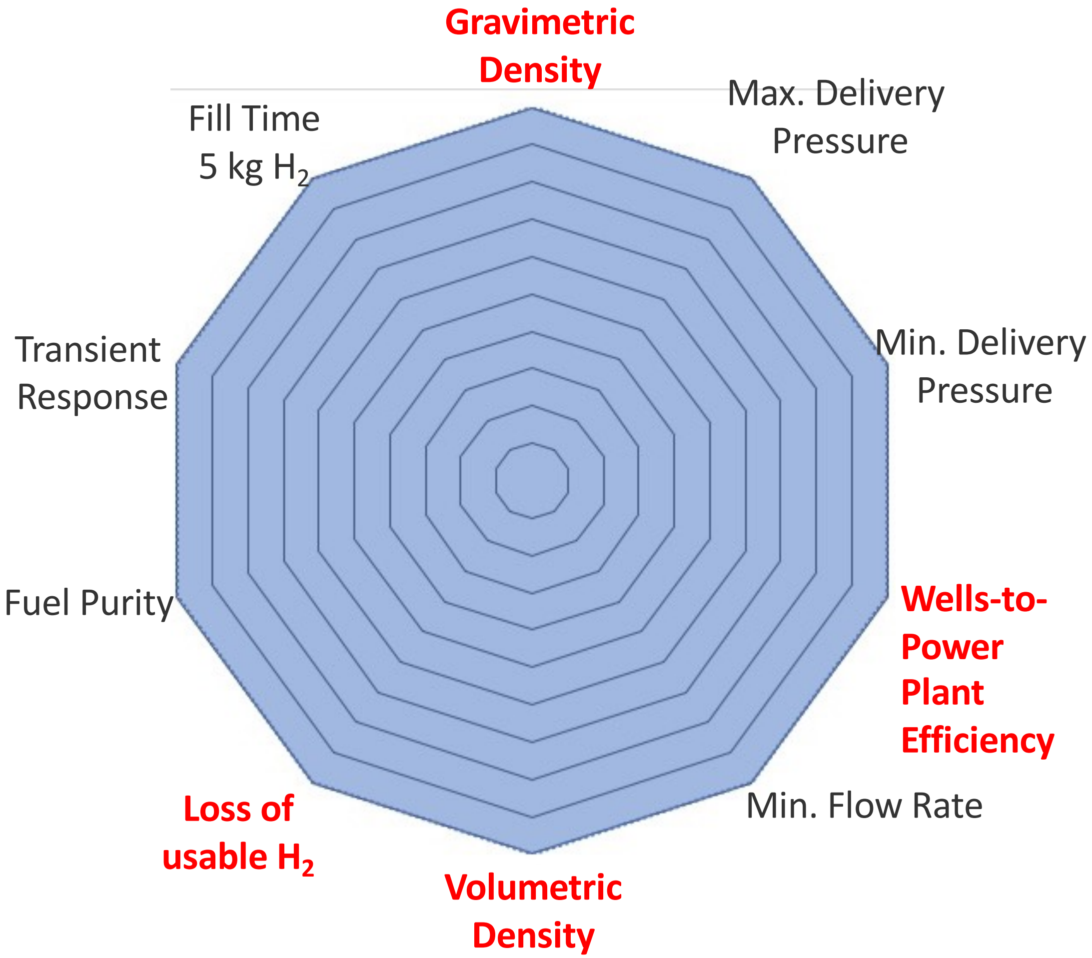
Volumetric/gravimetric capacity

- Bind multiple H_2 to open metal sites
- Sol-gel, compaction, particle shape control methods
- Design structurally dynamic MOFs

Operating temperature

- Functionalize MOFs to add strong-binding sites
- MOFs with metals in low oxidation states (e.g. V(II))

DOE Targets we are focusing on are shown in **red**



Approach Sorbents Phase 2 Focus Areas: the path forward

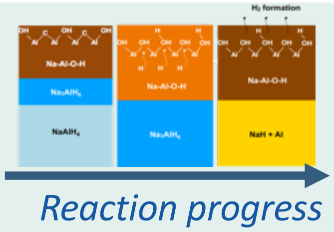
		DOE Targets				
	Focus Area project	Grav. Capacity	Vol. Capacity	Min. Deliv. T	Min. Deliv. P	Team*
	Enthalpy/Entropy under practical conditions			X	X	LBNL, NREL, PNNL
Adsorption energy to strong-binding sites	Electronic structure computations	X	X			LBNL
	Synthesis: π-basic metals	X	X			LBNL
	Synthesis: B/N Doping	X	X			NREL, PNNL
	Synthesis: highly polar open frameworks	X	X			NREL, LBNL
Sorbent packing	MOF monolith synthesis		X			LBNL, SNL
	Packing protocol		X			NREL
Dynamic sorbents	Flexible MOFs		X		X	LBNL, NREL
	Thermal/photo-responsive sorbent matrices		X		X	NREL, LBNL
	Multiple H_2 binding			X	X	LBNL, NREL, NIST
	Nanoscale defects in sorbents	X	X			SNL, NREL, LBNL

*Team lead is underlined

Hydrides Phase 1 Accomplishments: moved the bar toward materials that meet DOE targets

Min. operating T, P: Oxygenated surface species role in dehydrogenation

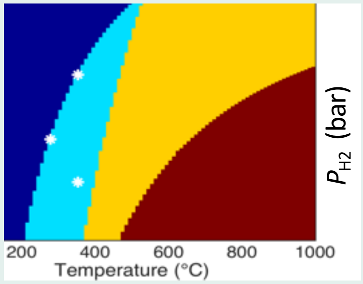
→ *Paradigm shift in understanding of hydride surface chemistry*



Min. operating T, P: comprehensive phase diagram for $Mg(BH_4)_2$

$\Delta H^\circ = 48$ kJ mol^{-1} (HSECoE target is 27 kJ mol^{-1}) →

→ bulk $Mg(BH_4)_2$ cannot meet DOE target



Min. flow rate: $Mg(BH_4)_2$@Carbon H_2 desorption T reduced by >100 °C

→ *Borohydride activation energy reduction by nanoscaling*

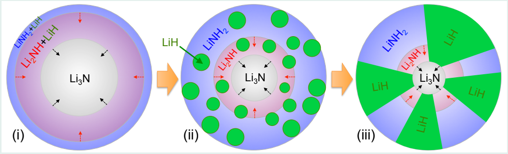
Gravimetric capacity: $Mg(BH_4)_2$@rGO >10 wt%

→ *Record capacity for nanoencapsulated complex metal hydride*

Min. operating T: Li_3N@(6nm-C) H_2 delivery T reduced by >180 °C

Bulk (430 °C) → Nano (250 °C)

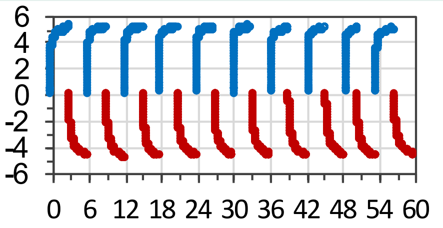
→ *Reaction path modification through nanointerface engineering*



Improved cycle life: Li_3N@(6nm-C) reversible >5 wt% H_2/250 °C/50 cycles

→ *Demonstrates durability of nanoscaled materials*

See also Slide 30 and ST132 for related information



Approach Hydrides Phase 2: building on Phase 1 discoveries

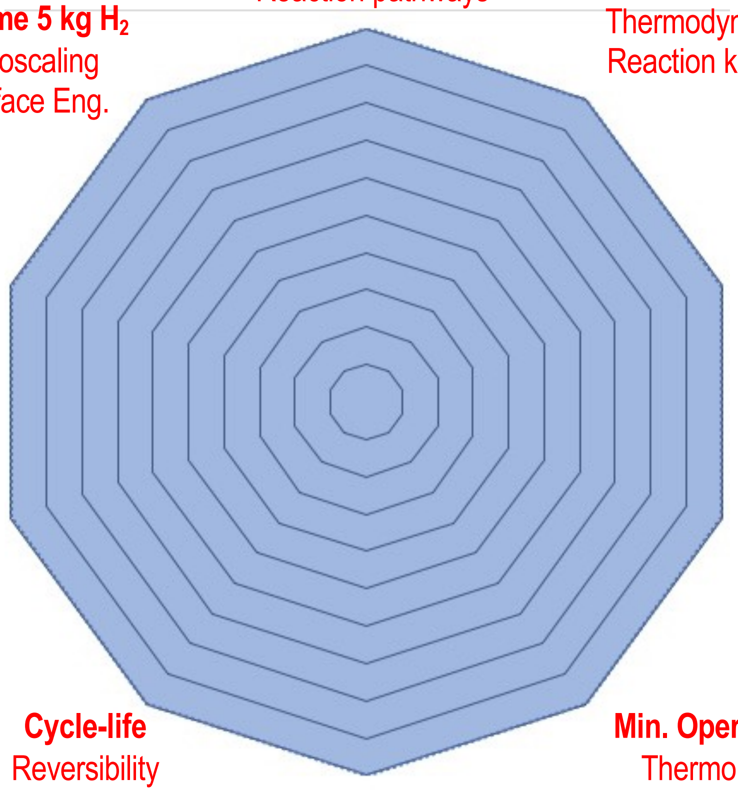
Science questions (selected)

- Are there undiscovered phases with favorable thermodynamics ≤ 27 kJ/mol H_2?
- Can nano-scale strain destabilize certain hydrides
- What are rate-limiting steps?

Strategies derived from Phase 1:

- Focus on relevant composition spaces
  - Borohydrides
  - Li-N-H
  - Ternaries (e.g. Li-B-Mg-H)
- Determine accurate phase diagrams
- Build on Phase 1 nanoscaling results
- Multiscale modeling to identify rate-limiting processes
- Target additives for specific bond activation
- Probe buried interfaces and surfaces using Phase 1 diagnostic tools
- Develop machine learning as new hydride material discovery capability

DOE Targets are interrelated but we are focusing on a key subset (shown in **bold**)



Gravimetric Density
Thermodynamics
Reaction pathways

Min. Deliv. P
Thermodynamics
Reaction kinetics

Fill Time 5 kg H_2
Nanoscaling
Interface Eng.

Start Time to Full Flow
Nanoscaling
Interface Eng.

Cycle-life
Reversibility
Side reactions

Volumetric Density
Packing density

Min. Oper. T
Thermo.
Kinetics

Approach Hydrides Phase 2 Focus Areas: the path forward

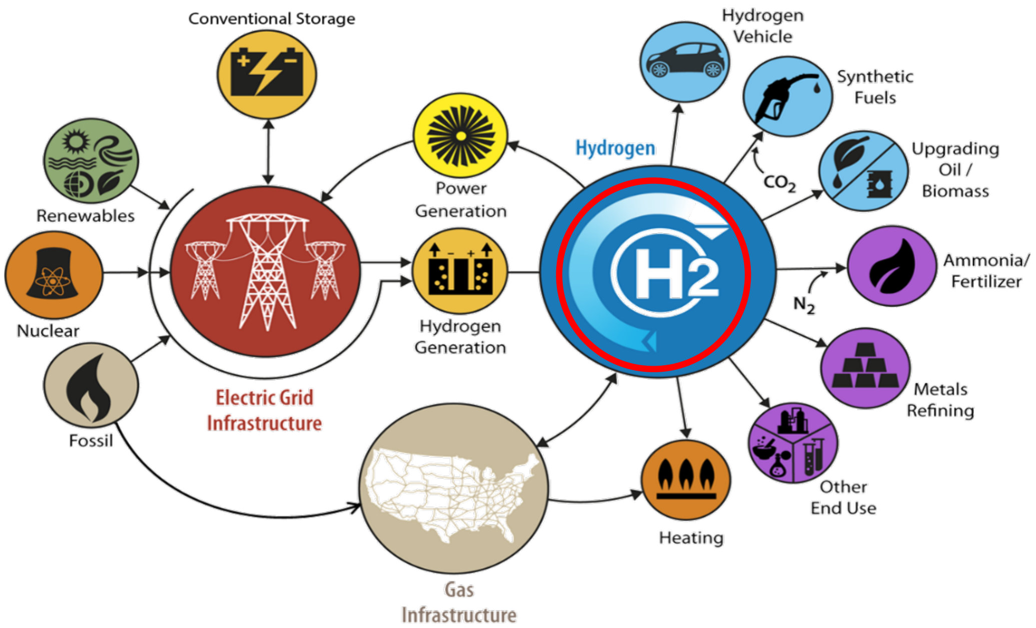
		DOE Targets							
	Focus Area project	Grav. Capacity	Vol. Capacity	Fill time	Time to full flow	Min. Deliv. T	Min. Deliv. P	Cycle life	Team (team lead is underlined)
Thermo.	Phase diagrams: ternaries	X	X			X	X		LLNL, SNL, PNNL
	Phase diagrams: eutectics	X	X			X	X		SNL, LLNL, PNNL, NREL
	Large-scale atomistic models	X	X	X	X				SNL, LLNL
Surfaces Interfaces	Interface Model Development			X	X			X	LLNL, PNNL, SNL
	Non-ideal surfaces; phase nucleation			X	X			X	SNL, LBNL, NREL, LLNL
Additives	Modulation of B-H bond strength			X	X	X			LBNL, NREL, PNNL
	Additives for B-B rehydrogenation			X	X	X			SNL, LLNL, LBNL, PNNL
	Modeling B-B/B-H catalytic activation			X	X	X			LLNL, SNL, LBNL, PNNL
Nano strategies	Nano-MH under mechanical stress			X	X				LLNL, NREL, LBNL, PNNL
	Non-innocent hosts see slide 31 & ST182			X	X				SNL, LLNL, LBNL
	MgB_2 nanosheets			X	X	X	X		LBNL, LLNL, SNL
	Microstructural impacts			X	X			X	LLNL, LBNL, SNL
	Machine learning	X	X						SNL, LLNL

Relevance: Hydrogen carriers: a new effort initiated in Phase 2

- **Bulk storage and transport are of central importance to the H2@Scale concept**
- **Highly varied storage needs:**
  - **Daily to seasonal in duration**
  - **Transport distances > 100s of km**

Goal: new concepts and materials that provide advantages over conventional compressed and liquefied hydrogen for bulk storage and transport

H2@Scale concept



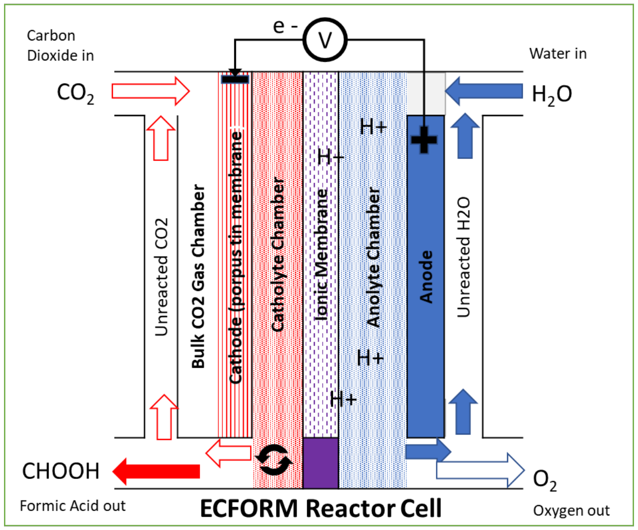
To learn more, see the HyMARC Hydrogen Carriers Webinar:
https://www.energy.gov/eere/fuelcells/downloads/hydrogen-carriers-bulk-storage-and-transport-hydrogen-webinar

Approach Hydrogen Carriers: Leverage capability and expertise in HyMARC consortium to accelerate progress

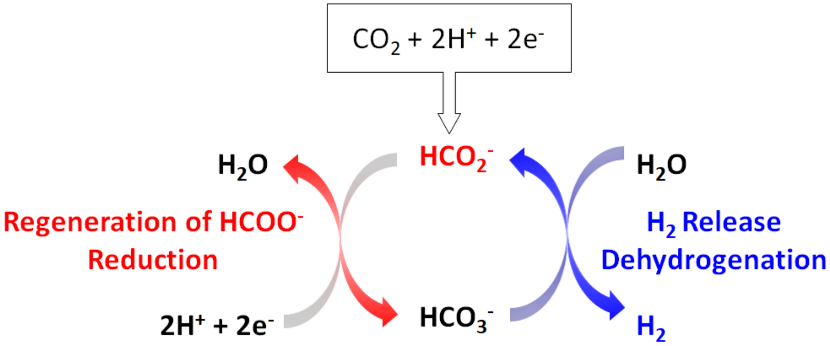
- **Metrics & targets:** Define the important properties of storage materials beyond onboard vehicular
- **Techno-economic analysis:** Determine advantages and limitations of materials and approaches to hydrogen carriers for transport and long-term storage
- **Novel material concepts: identify, characterize, and validate**
  - ○ Approaches to release or ‘adsorb’ hydrogen onto carriers
  - ○ No discrete step of making H_2(gas)
  - ○ Approaches to prevent phase changes
- **Catalysts: optimize the balance of properties:**
  - ○ Stability (Turnover number)
  - ○ Rates (Turnover frequency)
  - ○ Cost
  - ○ Selectivity
  - ○ heterolytic vs. homolytic H_2 activation

Examples of carrier strategies under consideration

Electrochemical approaches



Formate/bicarbonate cycle



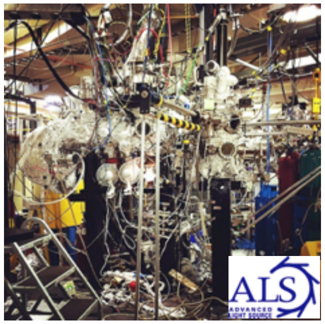
Approach Carriers Phase 2: nascent Focus Area projects

	Focus Area project	Team*
	Hydrogen carrier production without direct H_2 generation	PNNL
Liquid organic carriers	Dehydrogenative coupling in LOCs	PNNL
	Aqueous organic carriers	PNNL
	Liquid hydrogen carrier capacity determination	NREL
	Characterization methods and development	PNNL, NREL
	Eutectic systems	SNL, NREL, PNNL
Chemical carriers	Formate/bicarbonate cycle; formic acid (See slide 32)	PNNL
Adsorbents as carriers	Analysis of sorbents as hydrogen carriers	LBNL
	Porous liquids	NREL, LBNL
Novel material concepts	Bioinspired materials	NREL
	Plasmon interactions for "On-Demand" H_2 release	NREL, LBNL
	Heterolytic cleavage and H_2 activation	PNNL, NREL
	Catalyst stability	LLNL

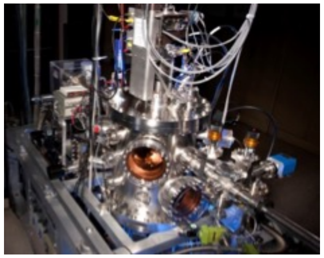
*Team lead is underlined

Phase 1 Accomplishment: comprehensive suite of characterization tools (in-situ, operando, all relevant length scales)

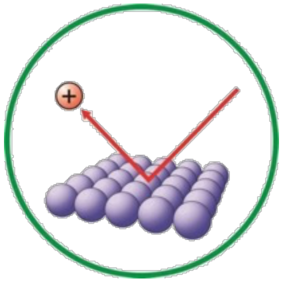
Atomic/molecular (0 – 1 nm)



AP-XPS
ALS/BL 11.0.2



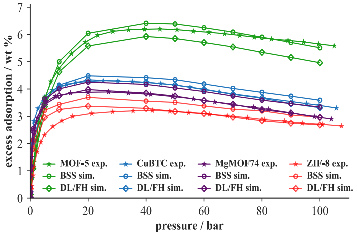
Lab-based AP-XPS

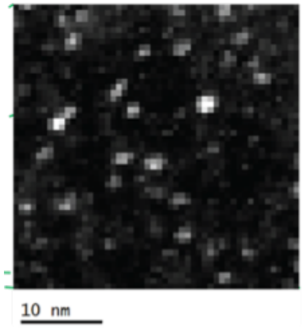


Low Energy Ion Scattering

Molecular/micro (0.5 – 2 nm)

Microporosimetry/BET

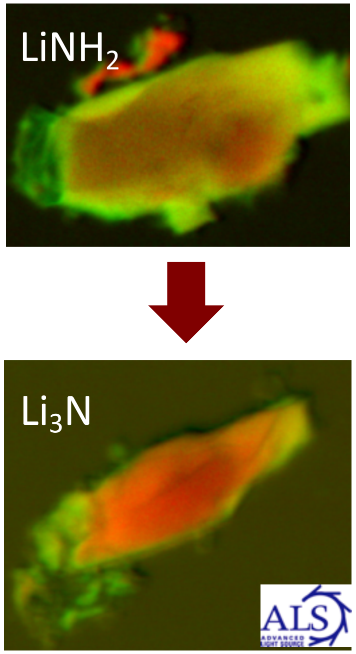




AC-TEM/STEM res. 63 pm

Mesoscale (2 - 100 nm)

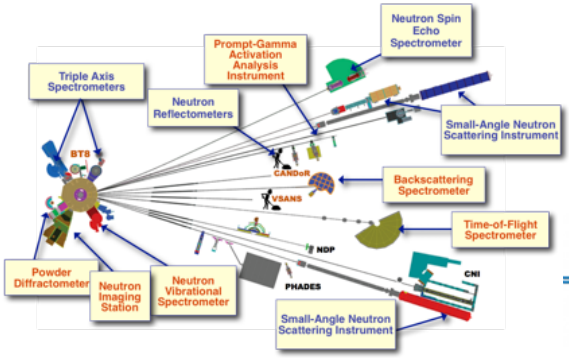
Grains (≤ 10 μm)



STXM (30 nm res.)

Neutrons:

- Spectroscopy
- Scattering
- Diffraction



NIST Center for Neutron Research

Macroscale/Bulk

Ultrahigh Pressure Reactor (1000 bar)

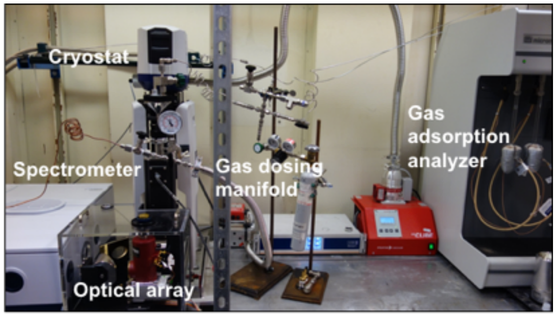
H-D exchange

10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2}

Length (m)

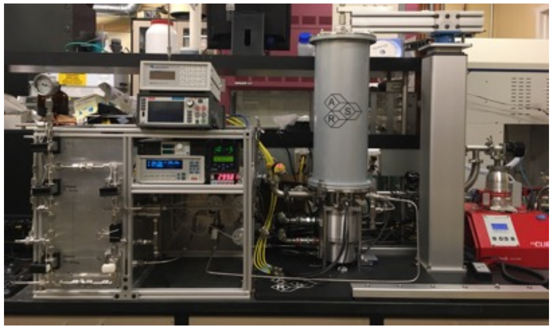
Phase 1 Accomplishment: extended characterization capabilities

DRIFTS



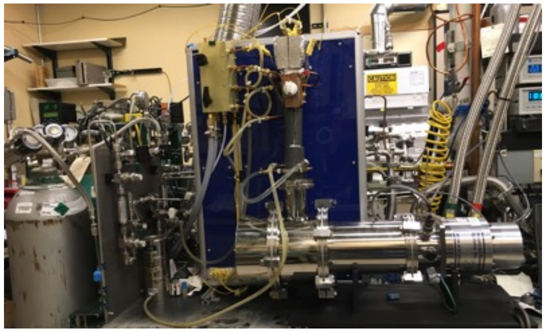
- Diffuse reflectance system coupled to cryostat and gas adsorption analyzer
- Can collect data at 15-373 K and 0-100 bar (controlled dosing up to 1.2 bar)

Thermal Conductivity



- H_2, He, CH_4, CO_2 from vacuum to 100 bar
- Temperature Range: 40 K to 375 K
- Sample types include solids & compressed pucks & powder

Variable Temperature PCT



- Modified PCT Pro system with capabilities of hydrogen pressures up to 200 bar, and a controlled temperature range from 40 – 350 K. (other gases possible including CH_4)
- New methodologies for increased measurement accuracy

P.A. Parilla et al. *Appl. Phys. A* **122** (2016), 201

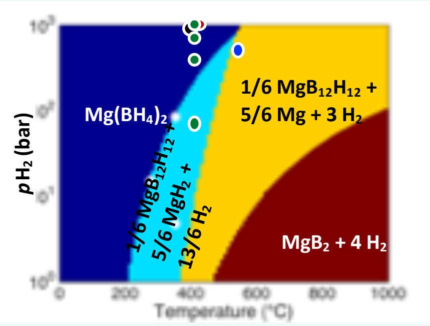
Approach Characterization Phase 2 Focus Areas: develop and enhance our Phase 1 advanced characterization capabilities

	Focus Area Topic	Team
	High-Temperature Validated PCT System	NREL, SNL
	PCT Calorimetry See slide 29 and ST131	NREL, PNNL
NMR	Advanced NMR: NMR-FTIR-PCT instrument	LBNL (Long)
	High-Temperature/Low-pressure NMR capability	PNNL (Bowden)
Advanced in-situ/ex-situ tools	Advanced in-situ, ex-situ Diffraction	SLAC, NIST
	Small-Angle X-ray Scattering	SLAC, NREL
	XAS/EXAFS	LBNL-ALS, SLAC
	Soft X-ray microscopies	LBNL-ALS
	Ambient-Pressure XPS	SNL, LBNL-ALS
	ATR DRIFTS for liquid carriers	LBNL
Neutron techniques	High-P/variable-T for Neutron Scattering Measurements	NIST
	Quasi-Elastic Neutron Scattering (QENS)	NIST
	VISION (highest resolution broadband INS	ORNL

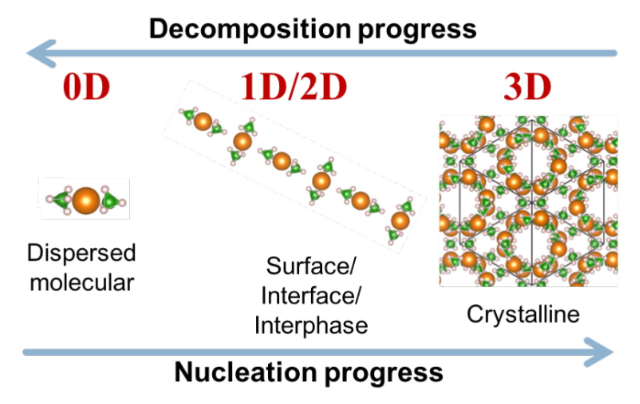
Phase 1 Accomplishment: Multiscale modeling from understanding to design

See ST129 for more information

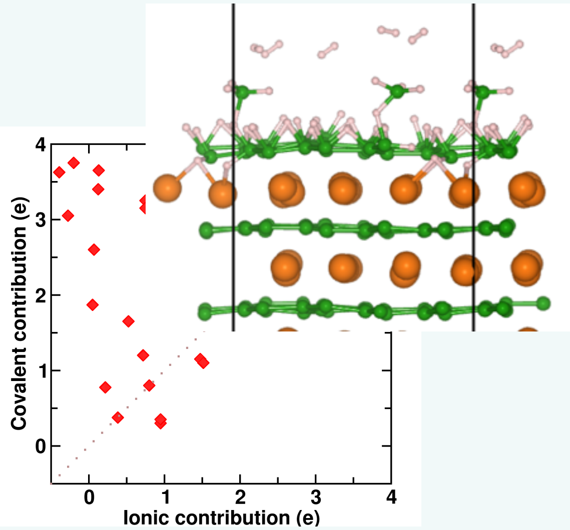
Predicting phase diagrams



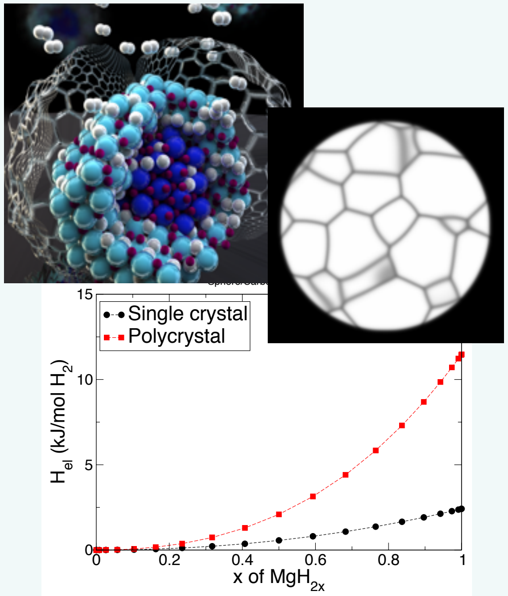
Simulating nucleation kinetics



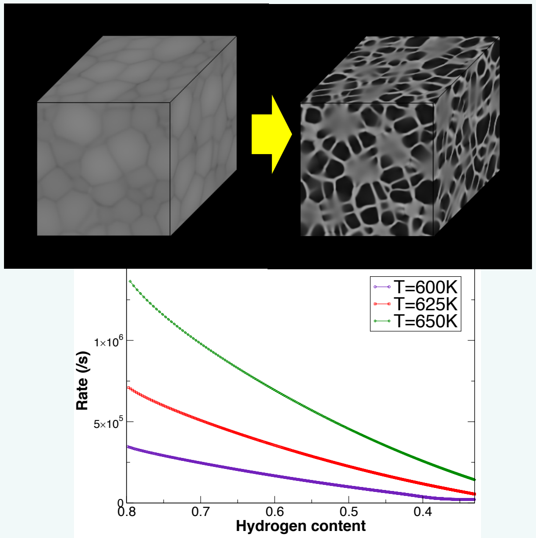
Understanding catalyst functionality



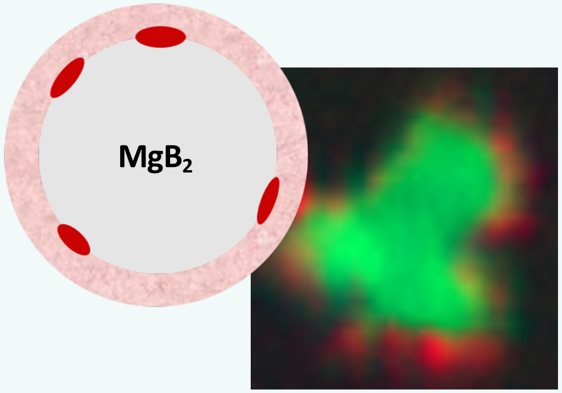
Assessing tunability via nanoconfinement



Direct modeling of isotherm uptake



Interpreting experiments



Collaboration & Coordination: HyMARC currently collaborates with Phase 2 Seedling

Seedlings: the HyMARC team assists individual projects with:

- **A designate HyMARC point-of-contact**
- **Technical expertise concerning specific scientific problems**
- **Access to HyMARC capabilities**
- ***Development of Magnesium Boride Etherates as Hydrogen Storage Materials*** (U. Hawaii)
  - Instability in MgB_2 B sheets explained (LLNL modeling investigation)
  - High-P hydrogenation, XRD, and FTIR performed for 43 MgB_2(etherate) samples
- ***Electrolyte Assisted Hydrogen Storage Reactions*** (Liox Power)
  - 1) High-P experiments and sample characterization; 2) Go/No-go tests
- ***ALD Synthesis of Novel Nanostructured Metal Borohydrides*** (NREL)
  - Nano-$Mg(BH_4)_2$ nanoparticle samples sent to NREL for ALD coating
- ***Optimized Hydrogen Adsorbents via Machine Learning & Crystal Engineering*** (U. MI)
  - Discussions on crystal engineering of OMS in MOFs

Selected international collaborations

- **Hydrides**
  - **KAIST Korea (Prof. Eun Seon Cho): strain-induced effects**
  - **Aarhus Univ. Denmark (Prof. Torbin Jensen): borohydrides**
- **Sorbents**
  - **Univ. Cambridge (Prof. David Fairen-Jamez): MOF consolidation methods**
- **Carriers**
  - **AIST (Prof. Qiang), *in–situ* solution NMR**

HyMARC Phase 2 Team Milestones

- **Milestone 1: 12/31/18:** Focus Area 6.1: Data Hub Determine HyMARC Data Needs: *Through meetings between the HyMARC Data Team and technical team members, we will identify data formats, sources and types used across HyMARC. We will develop best practices for data upload and sharing, and usage of defined metadata terms and forms.* **(100% complete)**

- **Milestone 2: 3/31/19**: Focus 3.D.2: Porous liquids as hydrogen carriers: *Porous Liquids: Demonstrate viability of click chemistry or nitrene approach for COF shell functionalization.* **(100% complete)**

- **Milestone 3: 6/30/19:** Focus 2.C: Activation of B-B and B-H bonds: *Demonstrate computational approach to enable screening of additives to activate B-B bonds in* MgB_2. **(in progress, on track)**

- **Milestone 4: 9/30/19:** *Demonstrate >6% reversible capacity for at least one Li-N-H or Mg-N-H phase, based on predicted composition from phase diagram, with reasonable kinetics at a temperature of ≤ 300 ˚C. PCT isotherm measurements will be carried out at temperatures ≤ 300 ˚C measuring total hydrogen uptake and release for each cycle. Isotherm plots and total hydrogen uptake and release data will be provided for each cycle. Data indicating at least 6wt% total hydrogen gravimetric capacity with reasonable kinetics at a temperature of ≤ 300 ˚C will constitute meeting the milestone criteria.* **(In progress)**

Proposed future work (Any proposed future work is subject to change based on funding levels.)

Project level

- Assess effectiveness of management structure and communications
- Evaluate progress of “applied” Focus Areas
- Renew Approved Program at LBNL/ALS for dedicated access to beam lines
- Establish access to VISION high-resolution instrument at ORNL/SNS

Data hub

- Begin uploading data to Data Hub, including DOE Hydrogen Storage Database

Sorbents

- Establish new models for determining isosteric heats and entropy from PCT data
- New methods for powder compaction, including gel formation and physical methods

Hydrides

- Activation of B-B and B-H bonds: *Demonstrate computational approach to enable screening of additives to activate B-B bonds in* MgB_2.
- Reversible capacity: Demonstrate >6% reversible capacity for at least one Li-N-H or Mg-N-H phase, based on predicted composition from phase diagram, with reasonable kinetics at a temperature of ≤ 300 ˚C

Carriers

- Carrier material approaches: Determine state-of-the-art

Advanced characterization

- Validate the new operational fluidized bed heated PCT System for temperatures up to 375 ˚C and pressures of 150 bar

Summary

HyMARC Phase 2 National Laboratory team continues these activities:

- Foundational research to accelerate materials discovery
- Development of advanced characterization tools
- Computational modeling across all relevant length scales
- Innovative material synthesis
- Innovative materials development
- Collaboration and assistance to Seedling projects

A new *Hydrogen Carriers* initiative was started (Tom Autrey, PNNL, lead)

A new Data Hub task was initiated (Kristin Munch, NREL, lead)

Organization/management structure revised:

- "Focus Area" projects developed to enable more agile, intensive research on specific areas
- Primary topic areas (e.g., Sorbents, Hydrides, etc.) have lead PI to ensure activities and progress remain on track

We are grateful for the financial support of EERE/FCTO and for technical and programmatic guidance from Dr. Ned Stetson, Jesse Adams, and Zeric Hulvey

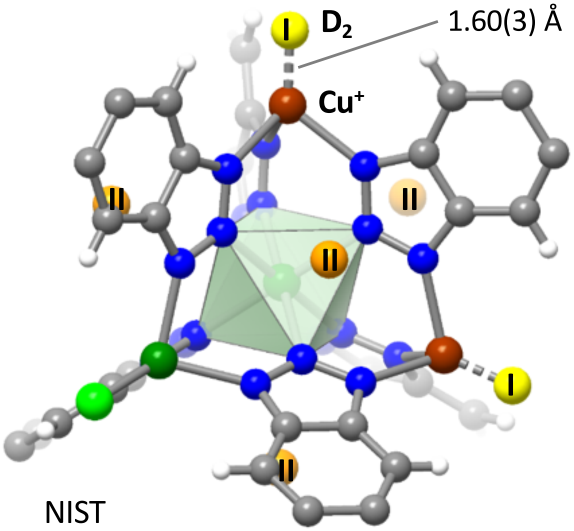
HyMARC

Hydrogen Materials Advanced Research Consortium

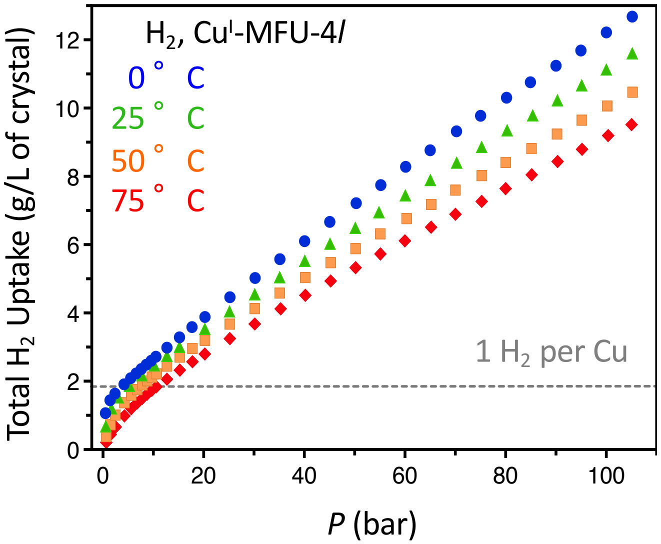
Enabling twice the energy density for onboard H_2 storage

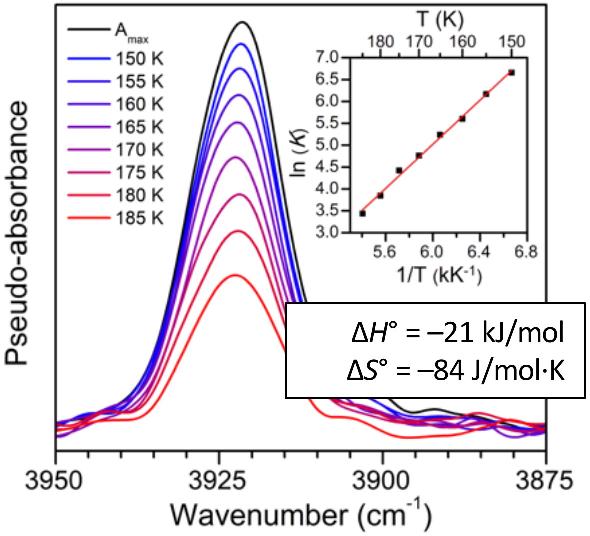
Technical Back-Up Slides

Increasing H_2 Binding Energies



NIST



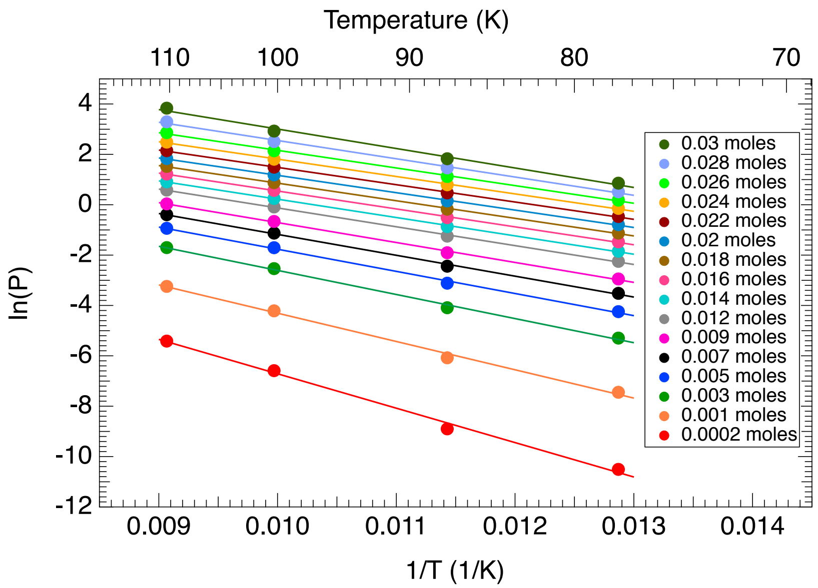


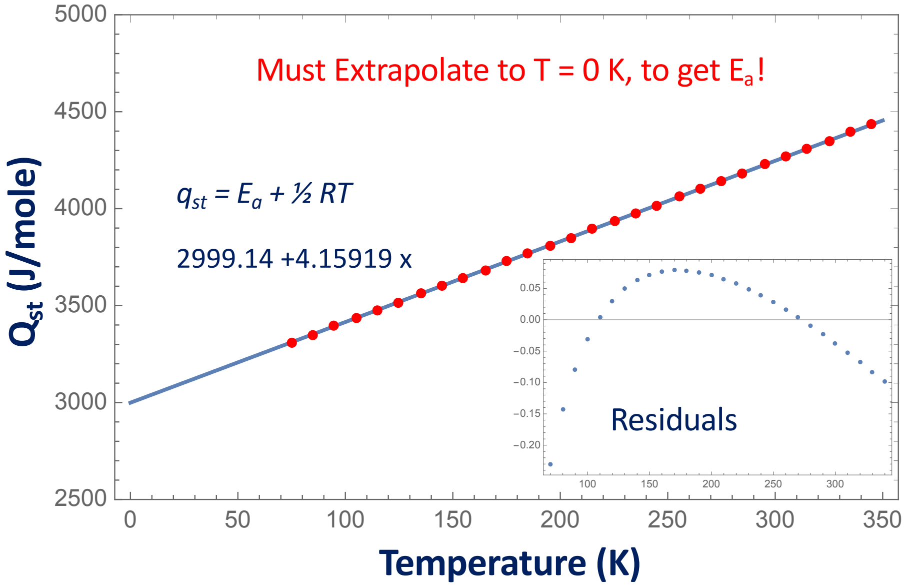
- ***In situ* powder neutron diffraction:** Extremely short Cu–D_2 distance observed in Cu^I-MFU-4*l* by neutron powder diffraction. Corroborates strong binding enthalpy and large red-shift of u(H–H) observed from DRIFTS.
- **High-P adsorption:** Open Cu^+ sites saturate at relatively low pressures. 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.

Thermodynamics and Isosteric Heats

- Milestone to determine Q_{st} at various T and to validate Cryo-PCT system completed in 2018
- Effort raised several issues about Q_{st} determination & motivated further investigation
- Modeling indicates that several types of bias can be introduced into this determination
- Fundamental assumptions are not valid in the supercritical state

Range from 9-6kj/mole





Must Extrapolate to T = 0 K, to get E_a!

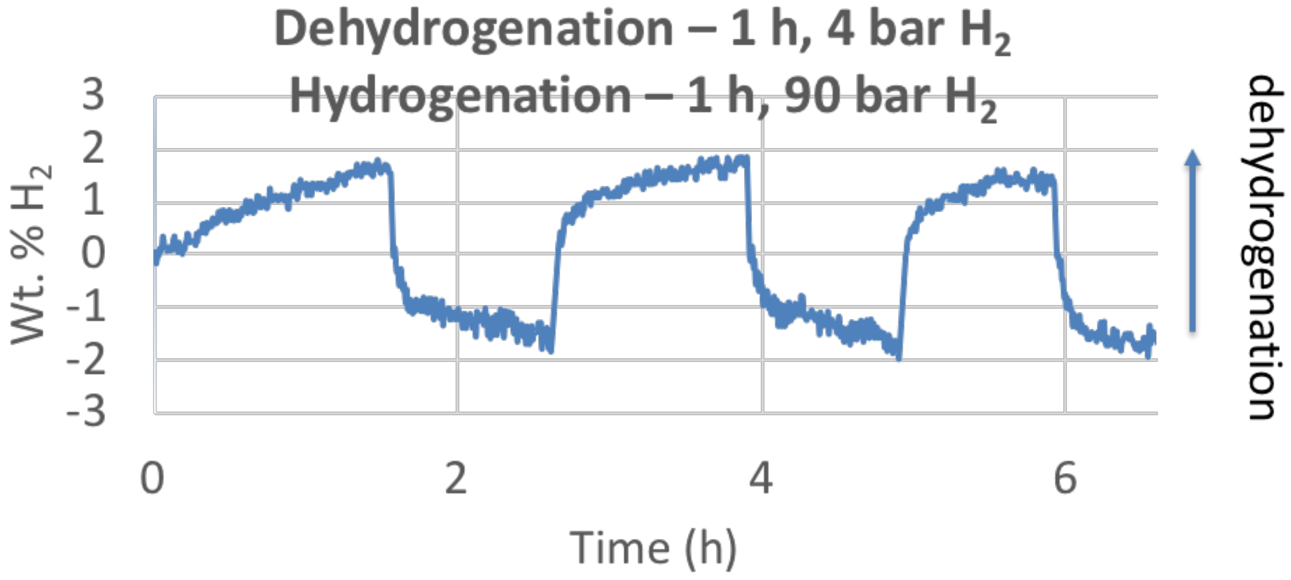
$q_{st} = E_a + ½ RT$

2999.14 +4.15919 x

Residuals

Highlight - Collaborative effort to understand the limitations to cycling $Mg(BH_4)_2 \Leftrightarrow MgB_{10}H_{10}$

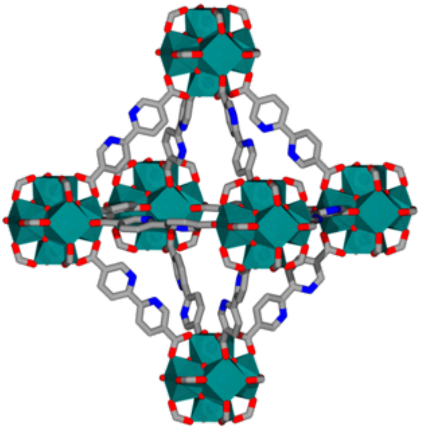
Thermodynamically feasible - but – how is it possible to reduce a closoborane, $MgB_{10}H_{10}$ to $Mg(BH_4)_2$ < 200 ˚C and < 100 bar H_2?



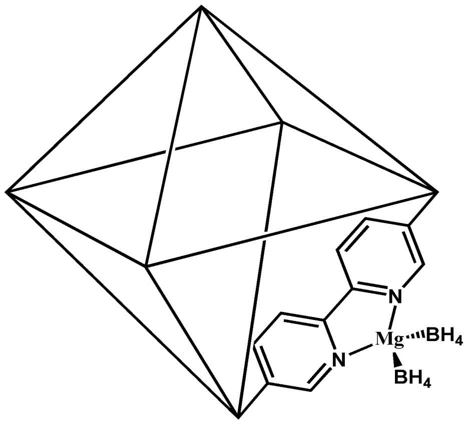
- **PCT cycling (Hawaii)**
- **TPD/MS and DSC (NREL)**
- **Synchrotron XR (Norway)**
- **NVS (NIST)**
- **In-situ NMR, XRD, IR, RAMAN, calc ΔG (PNNL)**
- **Solvent free (Geneva)**

- **Thermodynamics favor regen of $Mg(BH_4)_2$ from $MgB_{10}H_{10}$ (ΔH ca. 38 kJ/mol, ΔS ca. 95 J/K/mol, T (1 bar H_2) = 135 ˚C**
- **Additives, e.g., THF lower the mp of $Mg(BH_4)_2$.**
- **Sub-stoichiometric amounts, e.g., 0.25 THF/Mg results in a mixture of phases.**
- **Mixture melts between 75 – 100 ˚C to yield common amorphous phase.**
- **The melt amorphous phase is stable until ~ 180 ˚C, when H_2 is released to form $B_{10}H_{10}$ as the major product.**
- **Can do fast cycling, but heating too long or cooling to room temperature stops ability to cycle.**

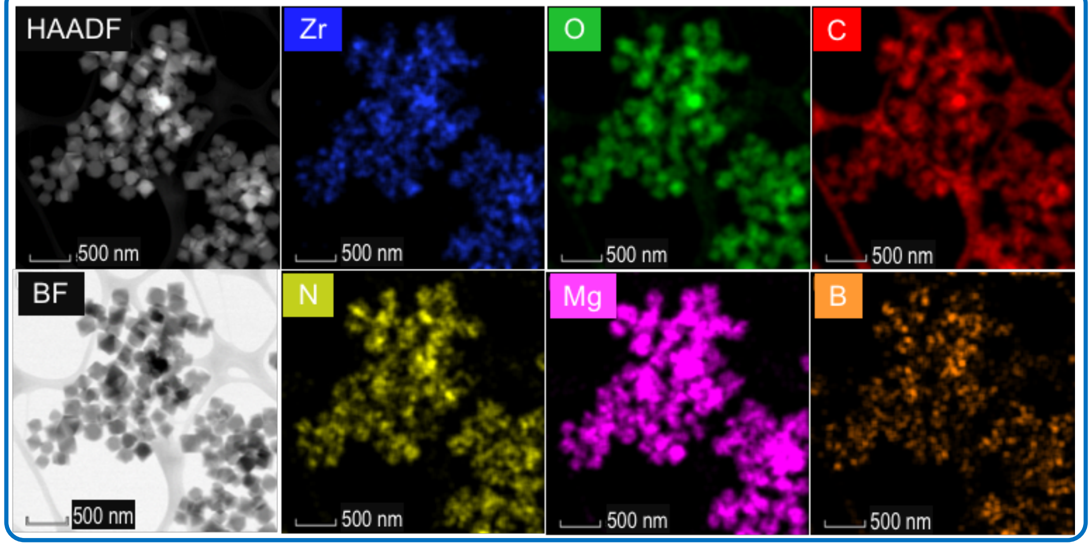
Isolated molecularly dispersed $Mg(BH_4)_2$ species with record low hydrogen release temperature

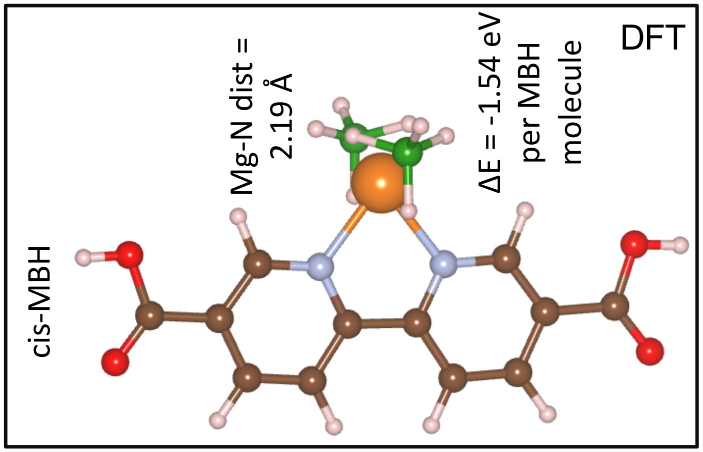


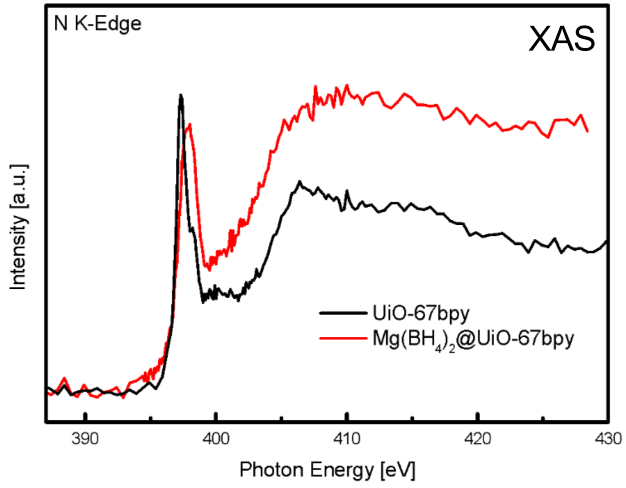
UiO-67-bipy

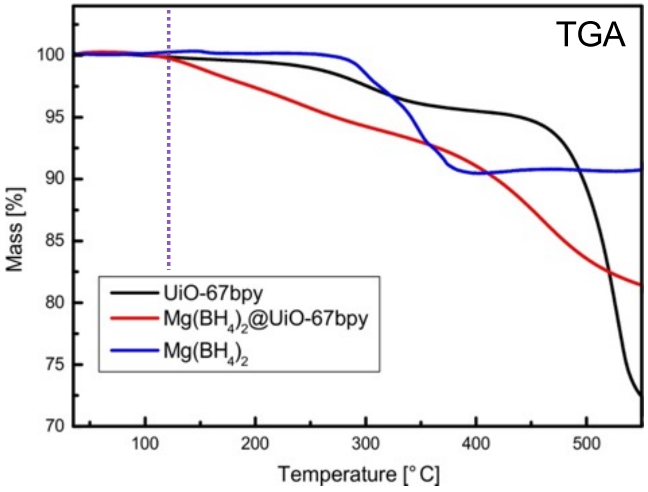


$Mg(BH_4)_2$@UiO-67-bipy









⇒ TEM and XAS data, coupled with DFT calculations, reveal that $Mg(BH_4)_2$@UiO-67-bipy is composed of molecular $Mg(BH_4)_2$ species coordinated to bipyridine groups

⇒ Hydrogen release starts as low as 120 deg. C, >100 deg. C lower than bulk.

Carrier concepts: Chemical compression from formic acid

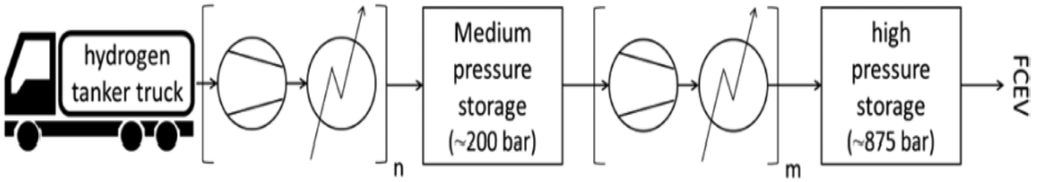
Max storage density ca. (FA) 53 g H_2/liter; generate >700 bar pressure

- Top challenges
  - Separation of H_2 from CO_2 at high pressure
  - Preparation of H_2CO_2 by electrochemical processes

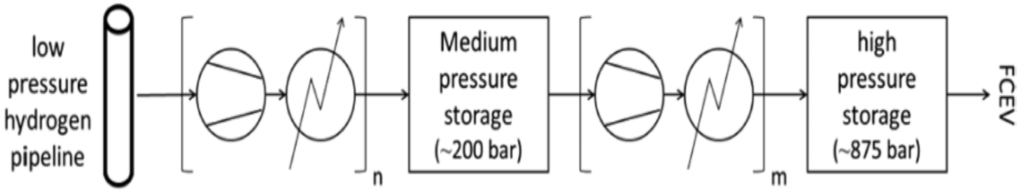
Collaboration with Karsten Mueller Hydrogenious

Schematics of various concepts for hydrogen fueling stations

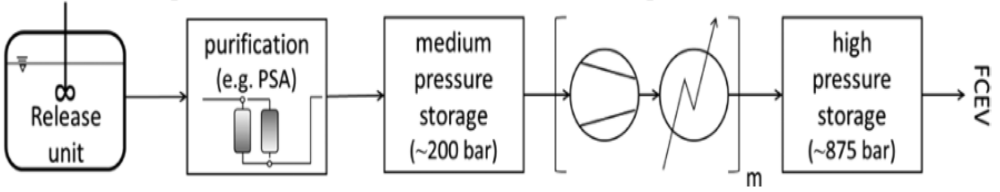
a) Schematic of a H_2 fueling station provided via trucks with pressurized hydrogen



b) Schematic of a H_2 fueling station based on a low pressure hydrogen source



c) Schematic of a H_2 fueling station using hydrogen carrier releasing H_2 at elevated pressures



Releasing Hydrogen at High Pressures from Liquid Carriers: Aspects for the H_2 Delivery to Fueling Stations

Energy & Fuels DOI:10.1021/acs.energyfuels.8b01724