

# HyMARC Core Activity: Metal Hydrides



*Enabling **twice the energy density** for onboard  $H_2$  storage*

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*This presentation does not contain any proprietary, confidential, or otherwise restricted information*

**Project ID: ST203**

# Task 2: Metal Hydrides

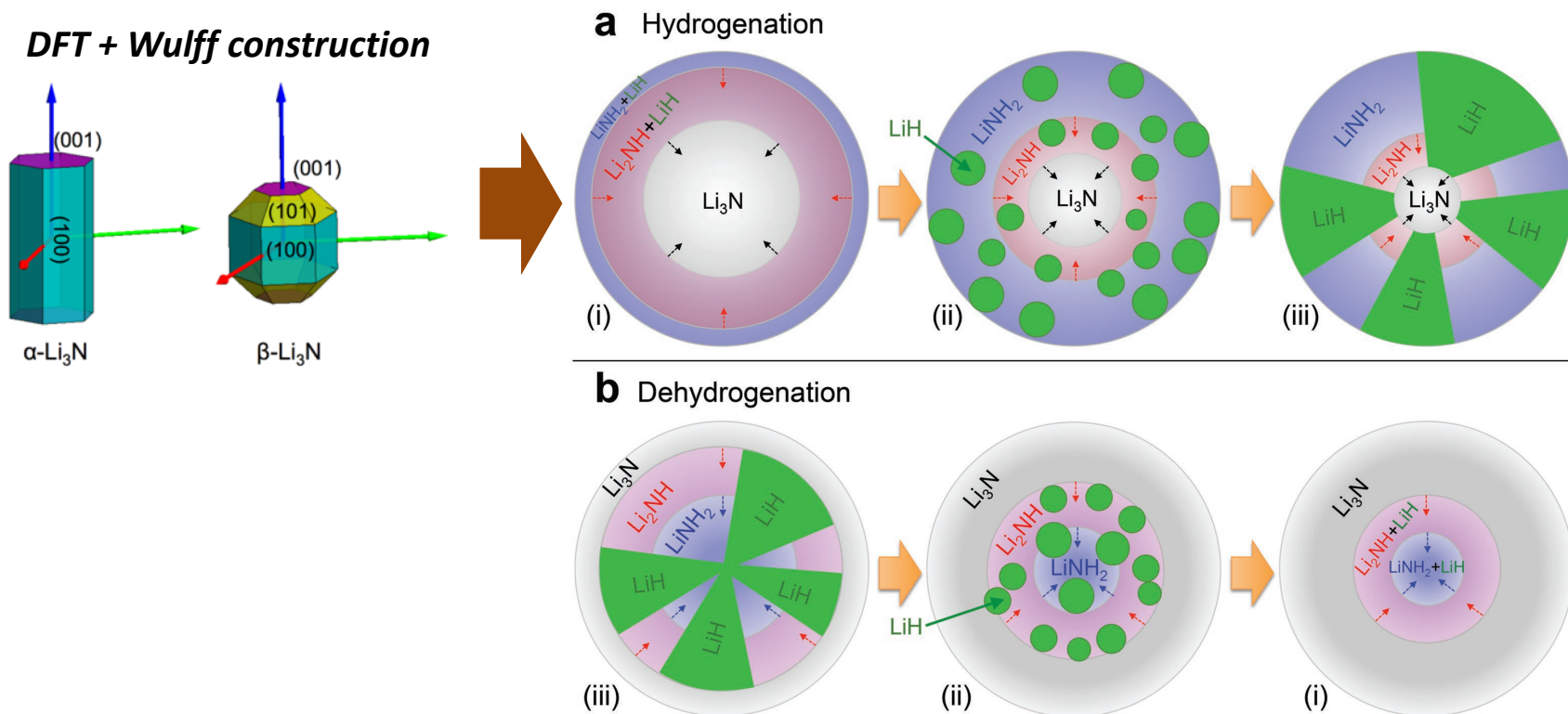
		DOE Targets							Team ( <u>lead</u> )	Status	
		Focus Area project		Grav. Capacity	Vol. Capacity	Fill time	Time to full flow	Min. Deliv. T			Min. Deliv. P
Surfaces & Interfaces	Thermo.	Phase diagrams: ternaries	X	X				X	X	<u>LLNL</u> , SNL, PNNL	Manuscript in progress
		Phase diagrams: eutectics	X	X				X	X	<u>SNL</u> , LLNL, PNNL,NREL	Continuing. New high-capacity eutectics in Li-Mg-B-N-H identified
		Large-scale atomistic models	X	X	X	X				<u>SNL</u> , LLNL	Mg-B-H forcefield completed. Extending work to unstable hydrides
		Interface Model Devel.			X	X			X	<u>LLNL</u> , PNNL, SNL	Continuing. MS in progress
		Surface chem & phase nucl.			X	X			X	<u>SNL</u> , LBNL, NREL, LLNL	Continuing. Paper <i>Adv. Mater. Interfaces</i> (2020)
Additives		B-H bond strength modulation			X	X	X			<u>LBNL</u> , NREL, PNNL	Continuing. Manuscript submitted.
		Additives for B-B rehydrogenation			X	X	X			<u>SNL</u> ,LLNL,LBNL,PNNL	No-go; manuscript in prep.
		B-B/B-H catalytic activation			X	X	X			<u>LLNL</u> ,SNL,LBNL,PNNL	No-go; manuscript in prep.
Nano strategies		Nano-MH/mechanical stress			X	X				<u>LLNL</u> ,NREL,LBNL,PNNL	Continuing. Manuscript submitted
		Non-innocent hosts			X	X				<u>SNL</u> , LLNL, LBNL	Continuing. Manuscript subm. on “molecular” complex hydride
		MgB <sub>2</sub> nanosheets			X	X	X	X		<u>LBNL</u> , LLNL, SNL	Prepared nanoscale Mg-B by surfactant ball milling. Manuscript in prep.
		Microstructural impacts			X	X			X	<u>LLNL</u> , LBNL, SNL	Manuscript in progress
		Machine learning	X	X						<u>SNL</u> , LLNL	Continuing. Explainable ML applied to interstitials. Paper published in <i>JPCL</i>

# Focus Area 2.B.2: Experimental probing of surface and buried interface chemistry of complex “non-ideal” systems

- Li-N-H is fully reversible (J. Wang *et al. MRS Bull.* 2013, 38, 480)
- Total capacity of ~10.5 wt.% via lithium imide ( $\text{Li}_2\text{NH}$ ) intermediate:



- Model of phase evolution based on kinetic data (B. Wood *et al. Adv. Mater. Interf.* 2017)

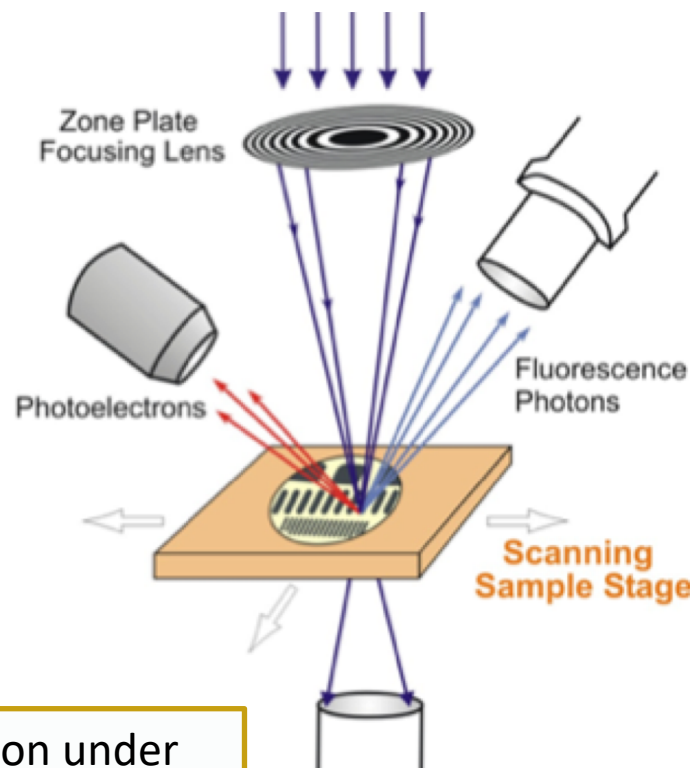


# Can we image phase evolution in metal hydrides?

*Uncovering the rate-limiting step in  $H_2$  uptake/release help us design materials with kinetics that meet DOE targets for fill time*

*Mesoscale phase evolution ( $nm \rightarrow \mu m$ ) is commonly included in mechanisms of metal hydride chemistry, but experimental data needed for validation is lacking.*

- TEM: ineffective because hydrides decompose under electron beams
- Scanning transmission X-ray microscopy (STXM)
  - Access through Approved Program at LBNL/Advanced Light Source
  - Generates **mesoscale chemical maps**
    - Beamline 5.3.2.2 allowed access only to N in this material
    - 30-nm resolution



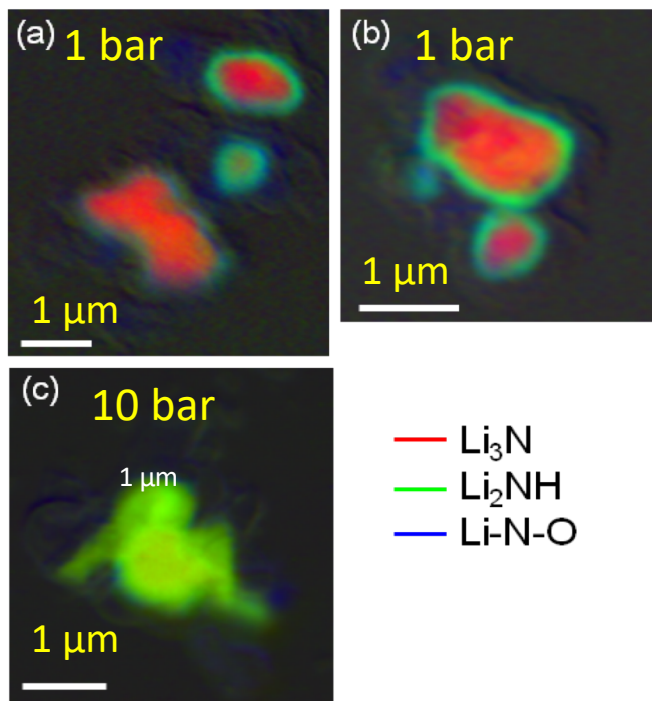
**Approach:** Conduct hydrogenation and dehydrogenation under realistic cycling conditions, then use clean transfer at the ALS to image at the mesoscale the reactants remaining and the products formed to understand the mechanisms of  $H_2$  storage reactions.



# STXM N K-edge maps of partially reacted $\text{LiNH}_2 + 2\text{LiH}$

## Hydrogenation

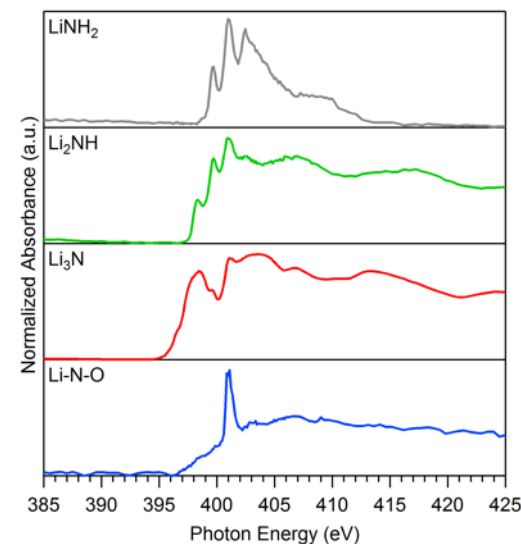
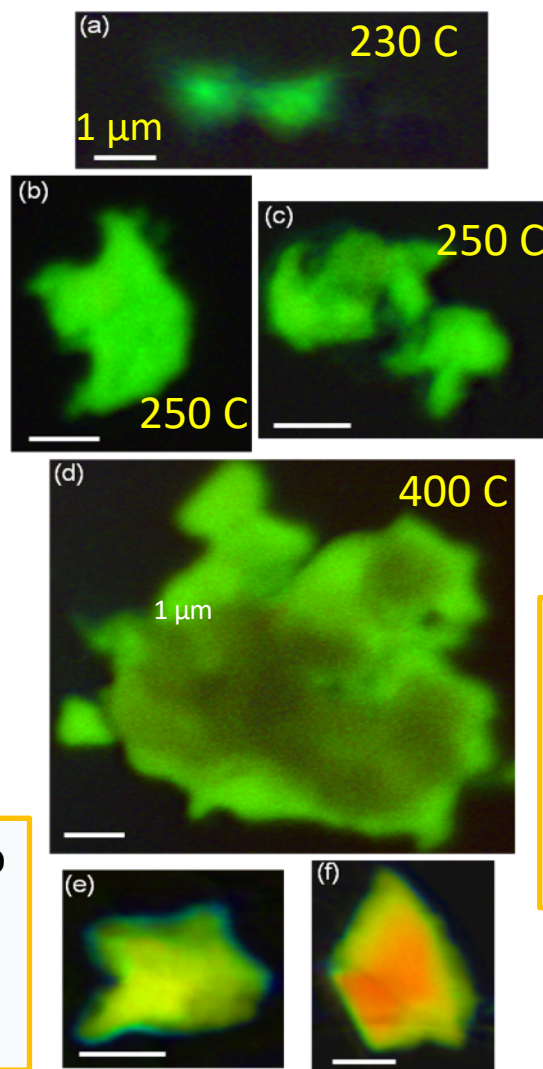
- Reaction at 200 C
- Very little  $\text{LiNH}_2$  detected



**Hydrogenation:** Bulk  $\text{Li}_3\text{N}$  starts to hydrogenate at the particle surface, with the imide growing into the particle center with time.

## Dehydrogenation:

- 400-450 C : Interior dehydrogenates first

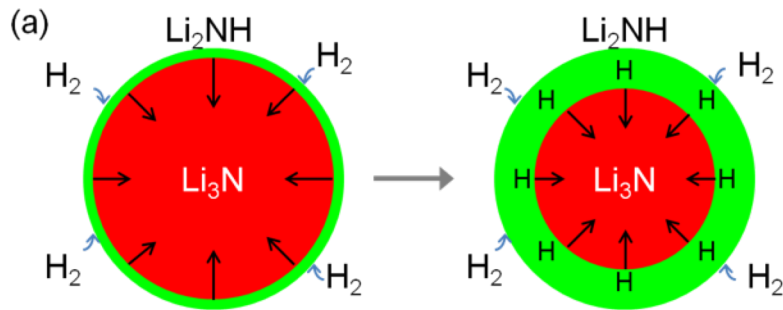


N K-edge X-ray absorption spectra, used as standards for mapping

**Dehydrogenation:** Bulk  $\text{Li}_2\text{NH}$  loses H from the interior of the particle first, which is counter-intuitive and currently being studied in more details.

# STXM maps indicate reaction is limited by the rate of $H_2$ release from the surface

Hydrogenation and dehydrogenation steps for complex metal hydrides are **conducted at different temperatures and pressures**, which can lead to different rate-limiting steps.

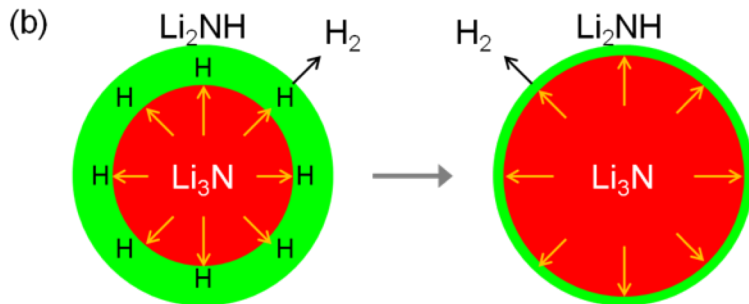


## Hydrogenation:

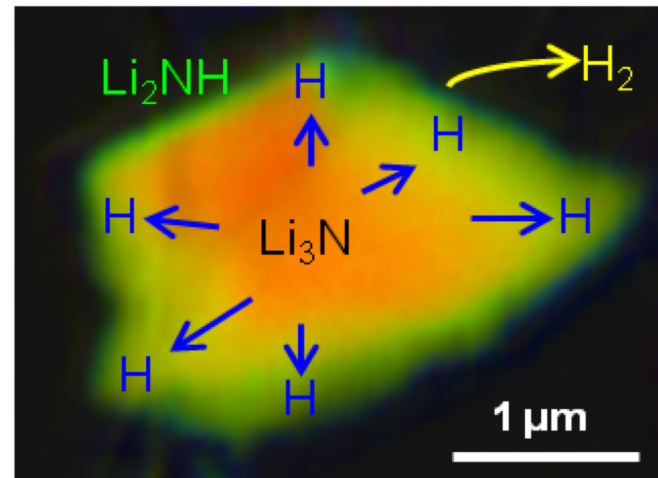
- Proceeds as predicted by Wood et al.

## Dehydrogenation:

- Slow surface kinetics lead to inverted core-shell  
→ opposite microstructure from earlier prediction

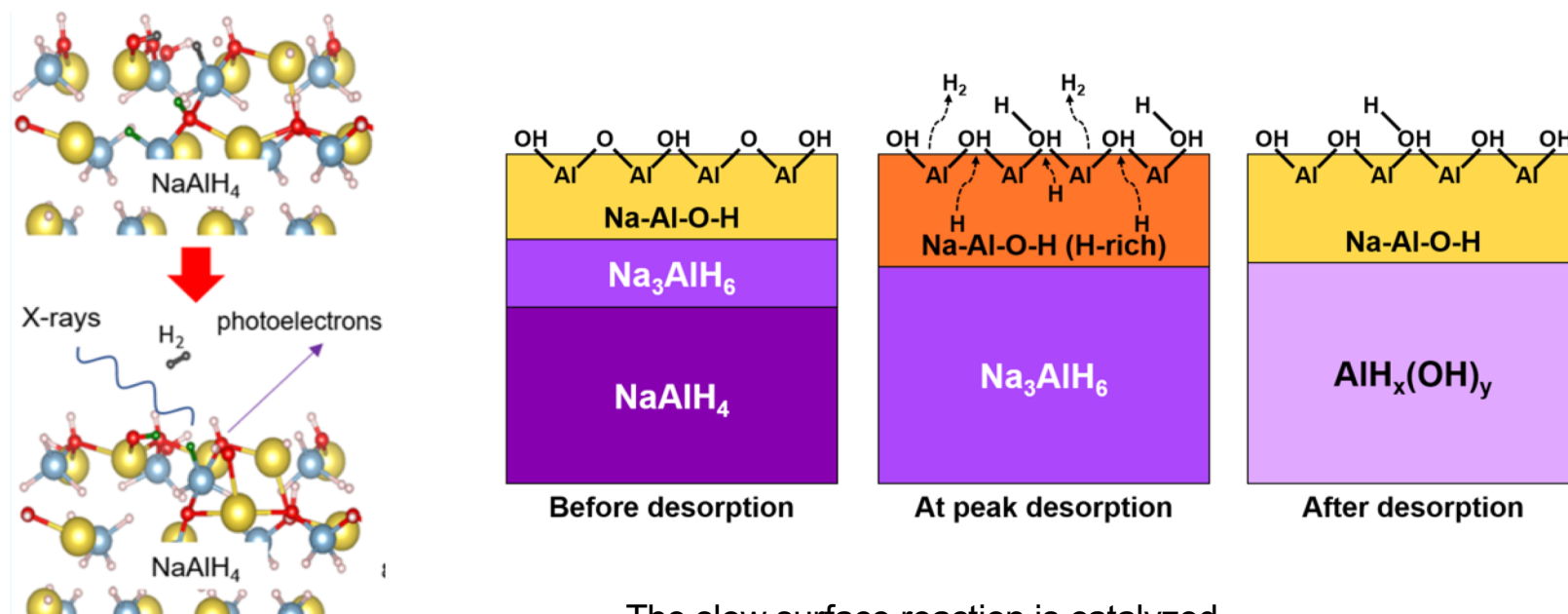


Inverted core-shell chemical map

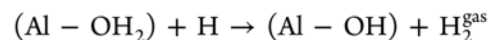


# In-situ Surface Characterization of NaAlH<sub>4</sub> dehydrogenation also suggests an inverted core shell mesostructure

*Finding emergent general behavior, such as inverted-core-shell dehydrogenation can improve model fidelity and provide guidance for designing, optimizing, or discarding new storage materials*

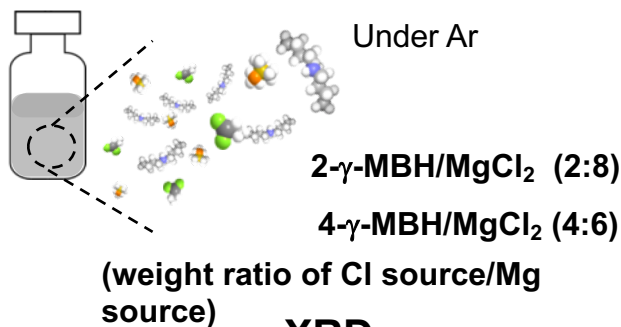


The slow surface reaction is catalyzed by activated surface Al (OH)<sub>x</sub>

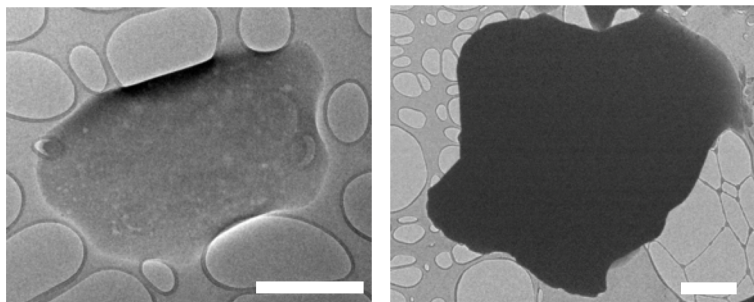


# Complex Metal Hydrides (eutectic mixtures)

## Solid-phase synthesis



## TEM images of 2- $\gamma$ -MBH/MgCl<sub>2</sub>



Size > 1  $\mu$ m

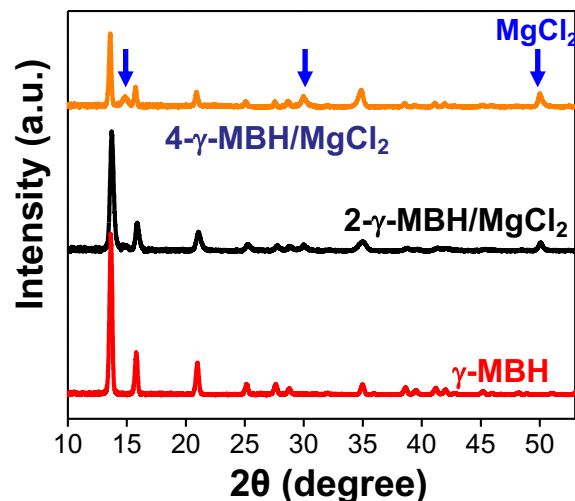
Scale bar: 500 nm

## Atomic ratio

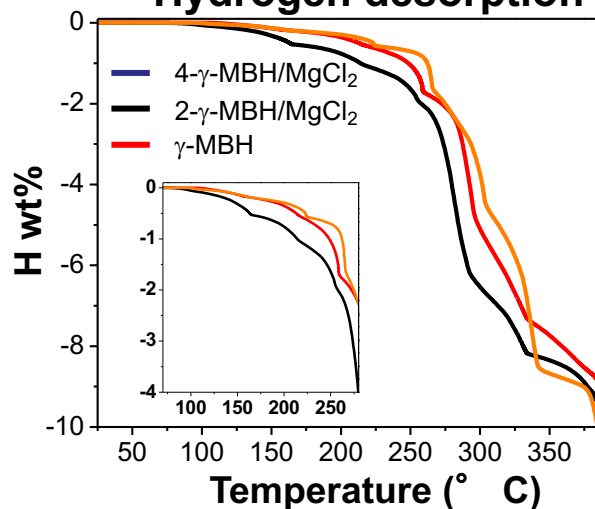
$$\begin{aligned} \text{B : Cl : Mg} \\ &= 6.3 : 1.5 : 2.1 \\ (\text{B+Cl}) : \text{Mg} &= 3.7 : 1.0 \\ &\text{*ideal : 2.0} \end{aligned}$$

Calculated by EDS data

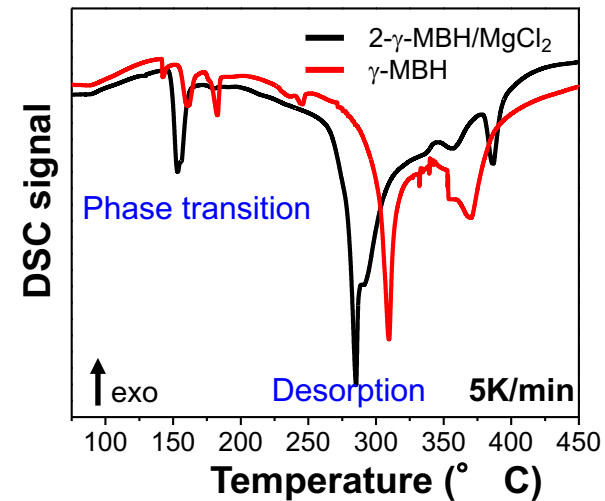
## XRD



## Hydrogen desorption



## DSC

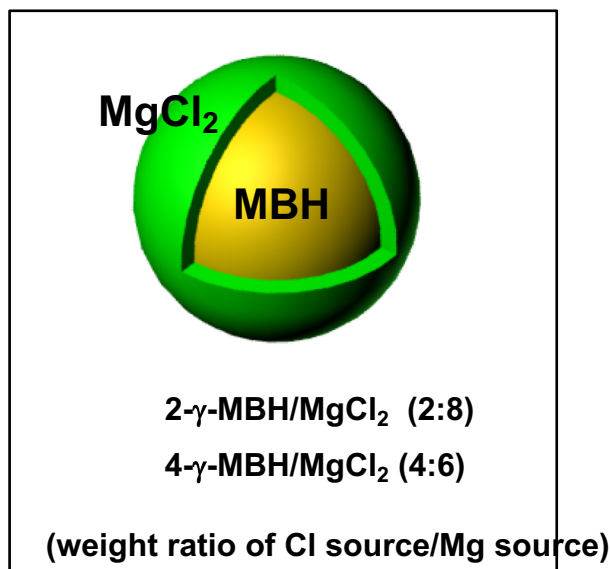


- Reducing the number of Mg cation in the mixture (perhaps by leaching Mg out to from MgCl<sub>2</sub>) might lead to increase probability of BH<sub>4</sub> interaction and release of H<sub>2</sub>.
- Dehydrogenation of 2- $\gamma$ -MBH/MgCl<sub>2</sub> starts at lowest temperatures among them.
- Phase transition and desorption in 2- $\gamma$ -MBH/MgCl<sub>2</sub> happen at lower temperature.

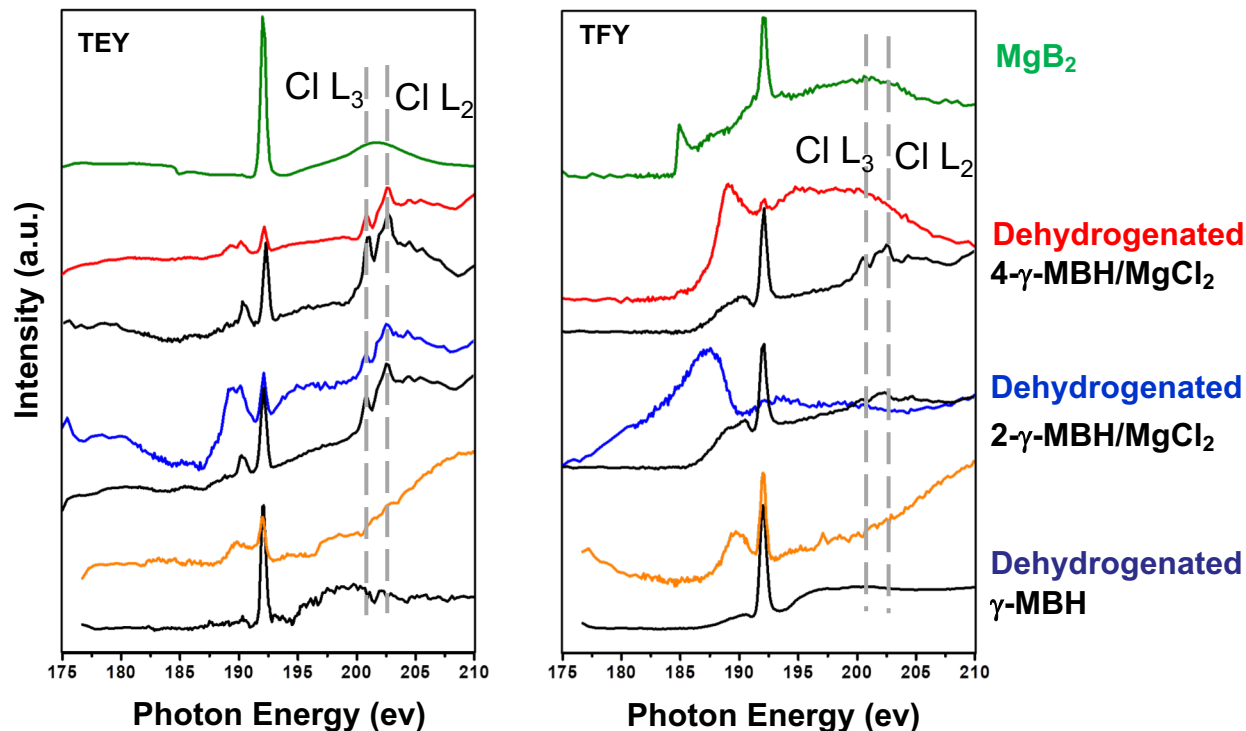


# B and Mg K-edge of XAS in eutectic mixtures

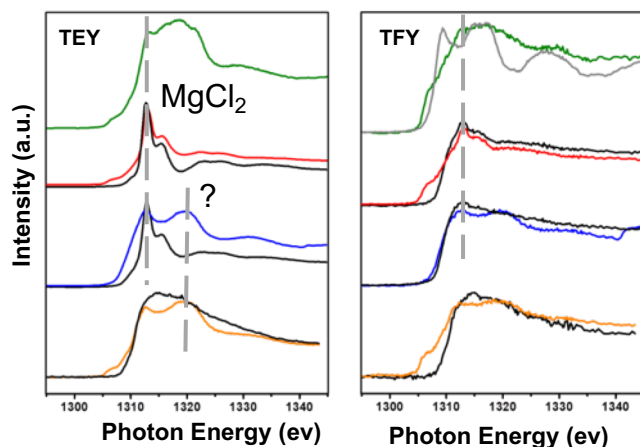
Surface and bulk analysis in as-synthesized and dehydrogenated mixtures



## B K-edge of XAS



## Mg K-edge of XAS



\*TEY: penetration depth: ~5nm \*TFY: penetration depth: ~ few micro

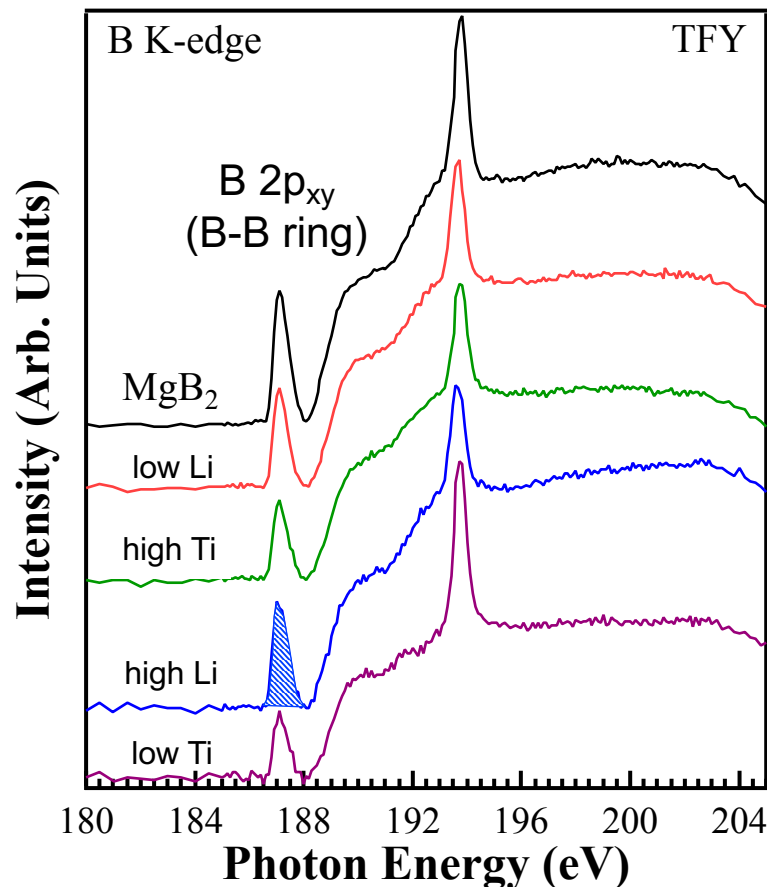
- MgCl<sub>2</sub> in 2-g-MBH/MgCl<sub>2</sub> is dominantly located on the surface.
- MgCl<sub>2</sub> might help to remove the oxygen in the bulk.
- Dehydrogenated 2-g-MBH/MgCl<sub>2</sub> in bulk does not show the peak corresponding to B<sub>2</sub>O<sub>3</sub>!

# Accomplishments: 2.C Activation of bonds in hydrides

## Understanding B-B bond disruption via additives, morphology changes

The B  $2p_{xy}$  intensity arises from the  $MgB_2$  B-B ring. LiH and  $TiH_2$  additives disrupt it.

“low” = 0.25 mole fraction; “high” = 0.47 mole fraction



Sample	Integrated B $2p_{xy}$ Area
$MgB_2$	0.44
$MgB_2$ + low Li	0.31
$MgB_2$ + high Li	0.36
$MgB_2$ + low Ti	0.20
$MgB_2$ + high Ti	0.25

Both Li and Ti reduce the B-B ring signal, but Ti disrupts it more (predicted by LLNL).

**Completed sample characterization by:**

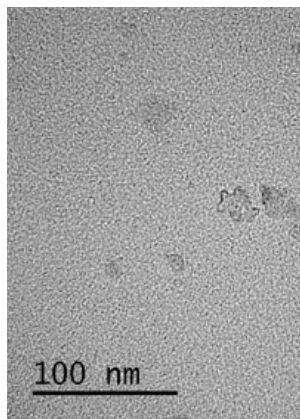
- ✓ XPS (LBNL)
- ✓ XAS (LBNL)
- ✓ XRD (SNL)
- ✓ FTIR (SNL)

**Approach:** We think  $MgB_2$  is hard to hydrogenate because of the stability of the B-B ring. Use additives to disrupt the B-B ring and see if hydrogenation improves.(in progress).

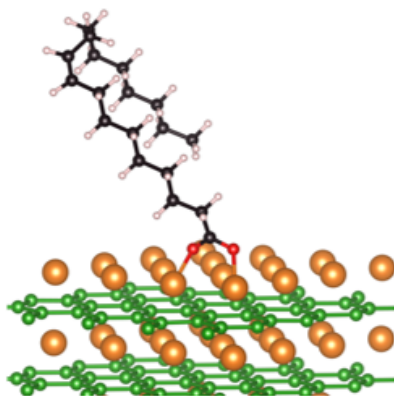
# Accomplishments: 2.C Activation of bonds in hydrides

## Understanding B-B bond disruption via additives, morphology changes

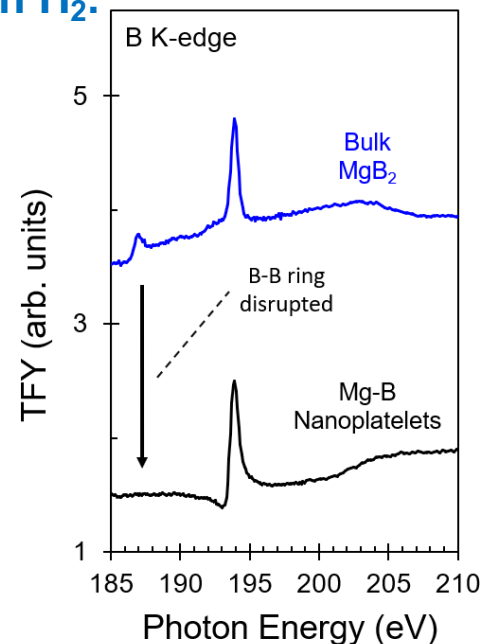
The morphology of  $\text{MgB}_2$  can be affected through surfactant ball milling, producing nanosheets of higher reactivity with  $\text{H}_2$ .



Oleate-bound nanosheets



Theory predicts oleate binding motif, properties



B K-edge XAS reveals the disruption of the B-B ring in the nanoplatelets.

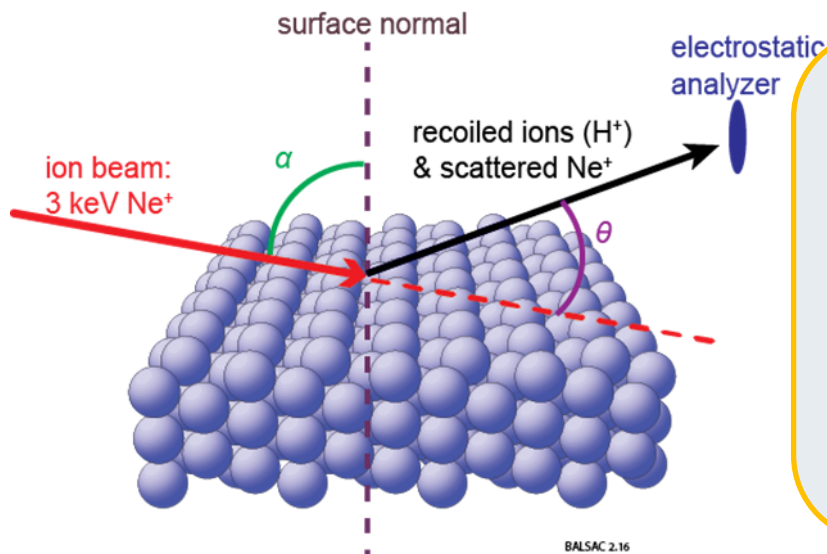
	Lattice Distortions Compared to Bulk $\text{MgB}_2$
In B-B plane, a (Å)	3.122 (+1.23 %)
□ to B-B plane, c (Å)	3.363 (-4.51 %)

XRD indicates lattice distortions from Bulk  $\text{MgB}_2$ , expanded within B-B nanosheets, contracted between them.

The Mg-B nanoplatelet material forms  $[\text{BH}_4]^-$  a full 100 °C below the threshold for  $\text{MgB}_2$  hydrogenation at 700 bar.

**Next Step:** Try to produce distorted Mg-B material without surfactant

# ARIES: Angle-Resolved Ion Energy Spectrometer



Ion beam (Ne<sup>+</sup>) is incident on surface at a glancing angle

Electrostatic analyzer detects ions:

- scattered Ne<sup>+</sup> (LEIS, low energy ion scattering)
- recoiled ions (DRS, direct recoil spectroscopy)

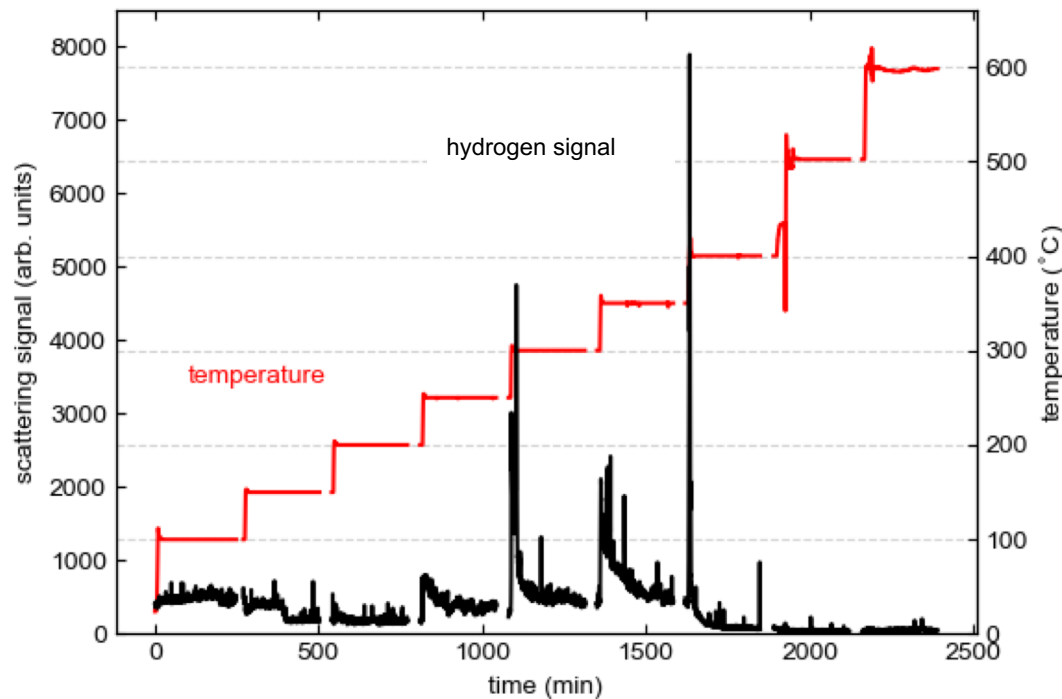
Energy of detected ions depends only on masses and  $\theta$ , providing surface composition information

## Key advantages of LEIS and DRS:

- Extreme surface sensitivity—first monolayer and adsorbates
- Direct detection of surface hydrogen (challenging for most surface science techniques)
- In-situ monitoring of surface in well-controlled environment ( $\sim 10^{-10}$  Torr, temperature control)



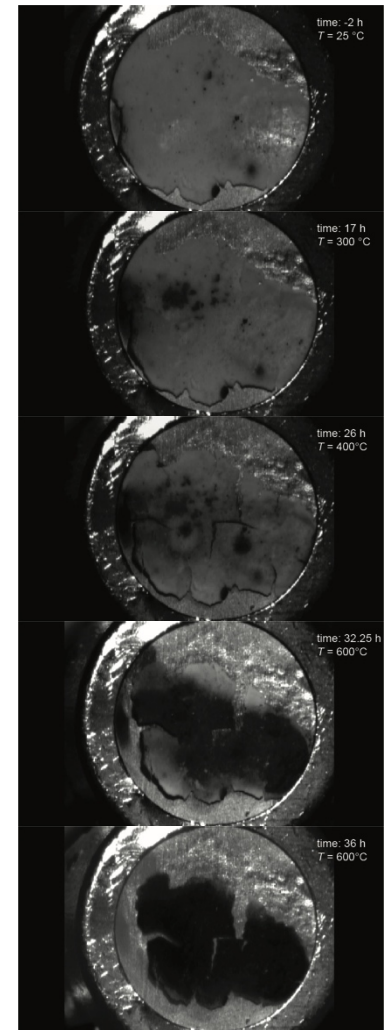
# ARIES surface evolution in $\text{Mg}(\text{BH}_4)_2$



Measurement of surface H with ARIES during the thermal decomposition of  $\text{Mg}(\text{BH}_4)_2$  pressed onto a gold foil:

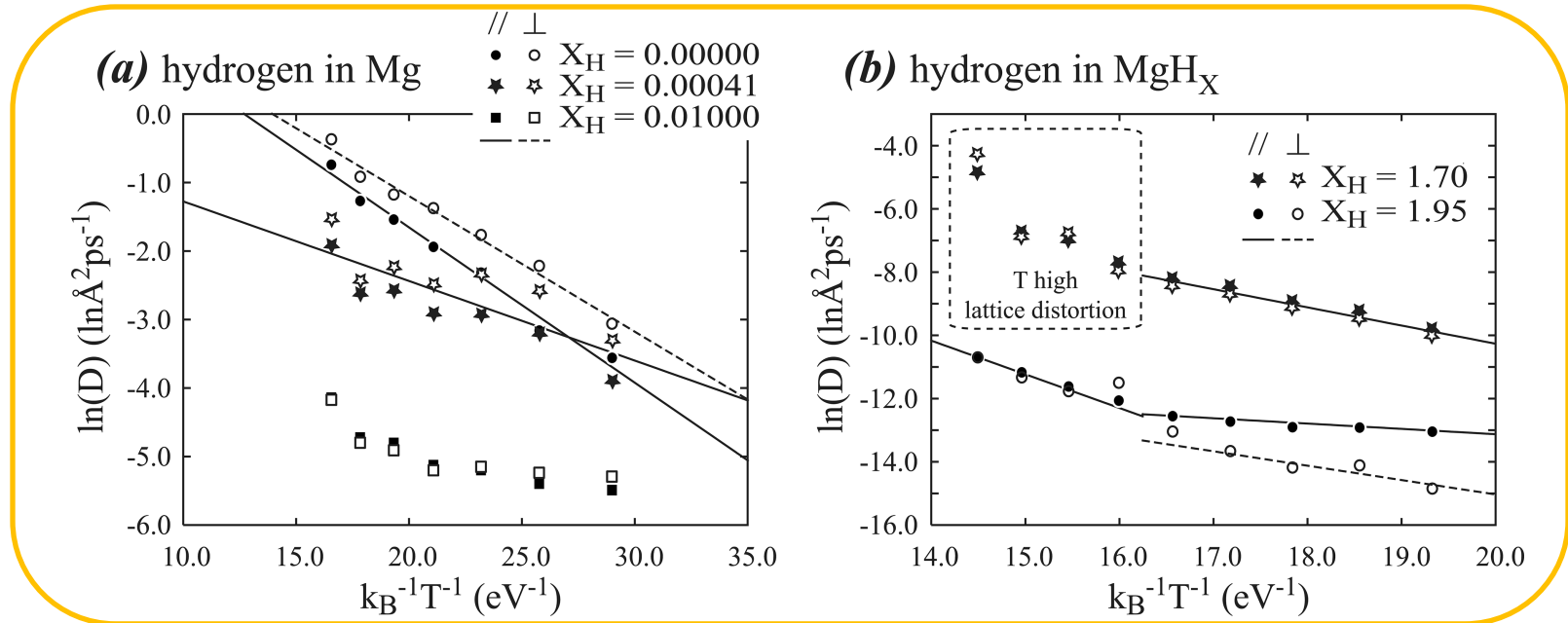
H segregated to surface mostly at 250-300 ° C and 350-400 ° C, in good agreement with TPD measurements in the literature [1]

[1] Soloveichik et al., Int. J. Hydrogen Ener., (2009).



# MD method for predicting H-diffusion in Mg and MgH<sub>2</sub>

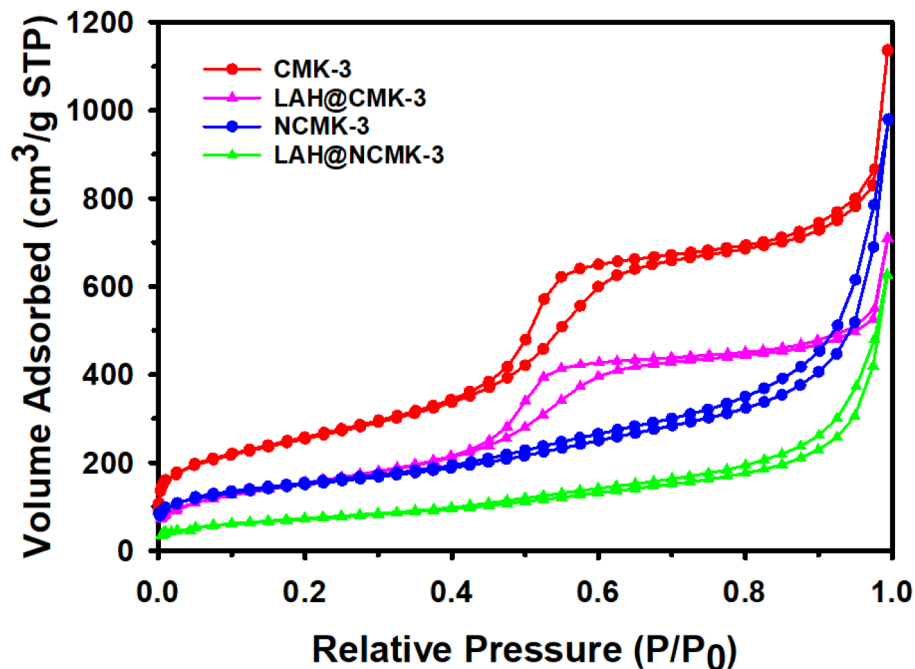
## Predicted Arrhenius Plots



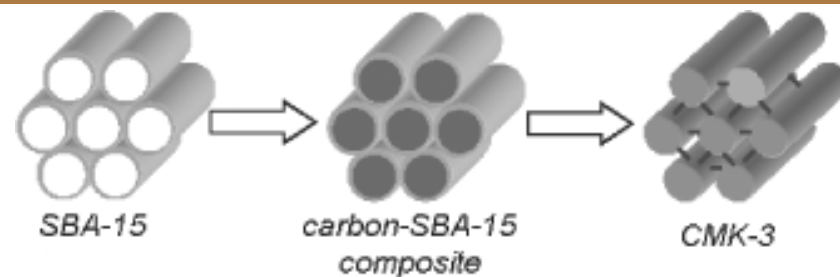
1. Joint SNL-LLNL effort to develop validated models of H-diffusion in Mg.
2. Experiments at given composition/phase cannot relate the diffusivities to hydrogenation state. Hydrogen atoms diffuse vastly faster in Mg metal compared to Mg hydride.
3. Simulations reveal predicted barriers of 0.22 eV in Mg and 1.1 eV in MgH<sub>2</sub>, values which agree with the 0.25 eV and 1.1 eV experimental values.

## Focus Area 2.D.2: Non-innocent hosts for metal hydride nanoencapsulation

### $\text{LiAlH}_4$ confinement within N-functionalized porous carbons



Nitrogen adsorption/desorption isotherms at 77 K of  $\text{LiAlH}_4$  infiltrated mesoporous carbon scaffolds

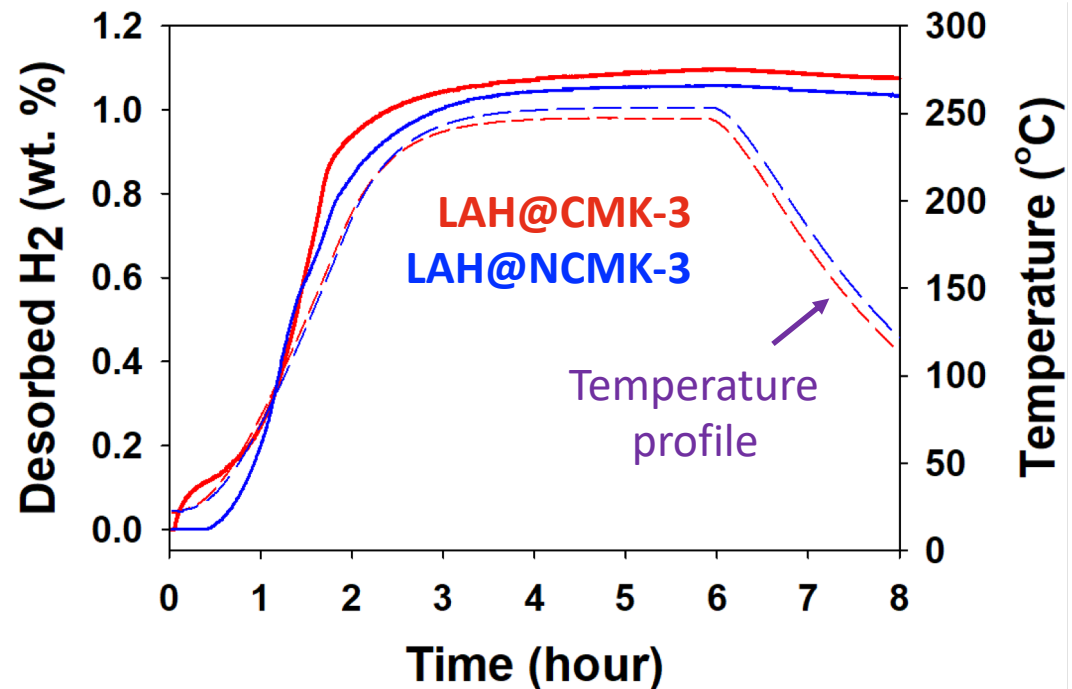
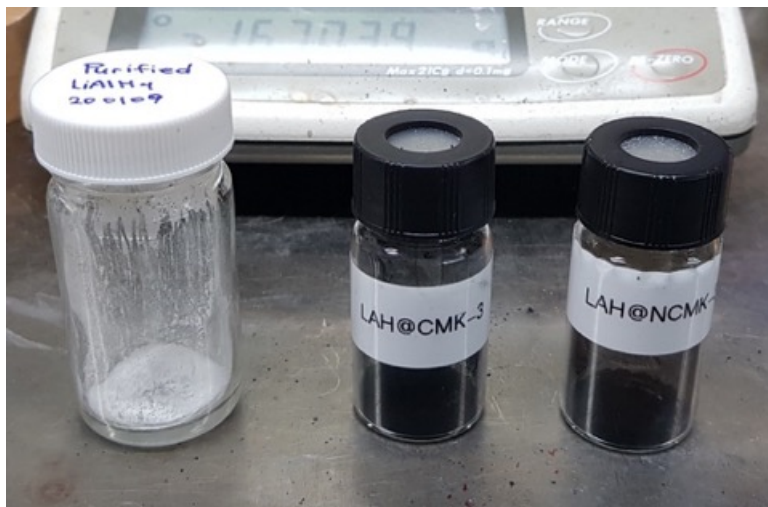


Sample	BET surface area ( $\text{m}^2 \text{g}^{-1}$ )	Total volume ( $\text{cm}^3 \text{g}^{-1}$ )
CMK-3	911	1.76
LAH@CMK-3	560	1.10
NCMK-3	534	1.51
LAH@NCMK-3	261	0.97

Summary of calculated BET surface area and total pore volumes with nitrogen adsorption / desorption isotherms

⇒ Successfully synthesized lithium alanate nanoparticles confined in CMK-3 carbons

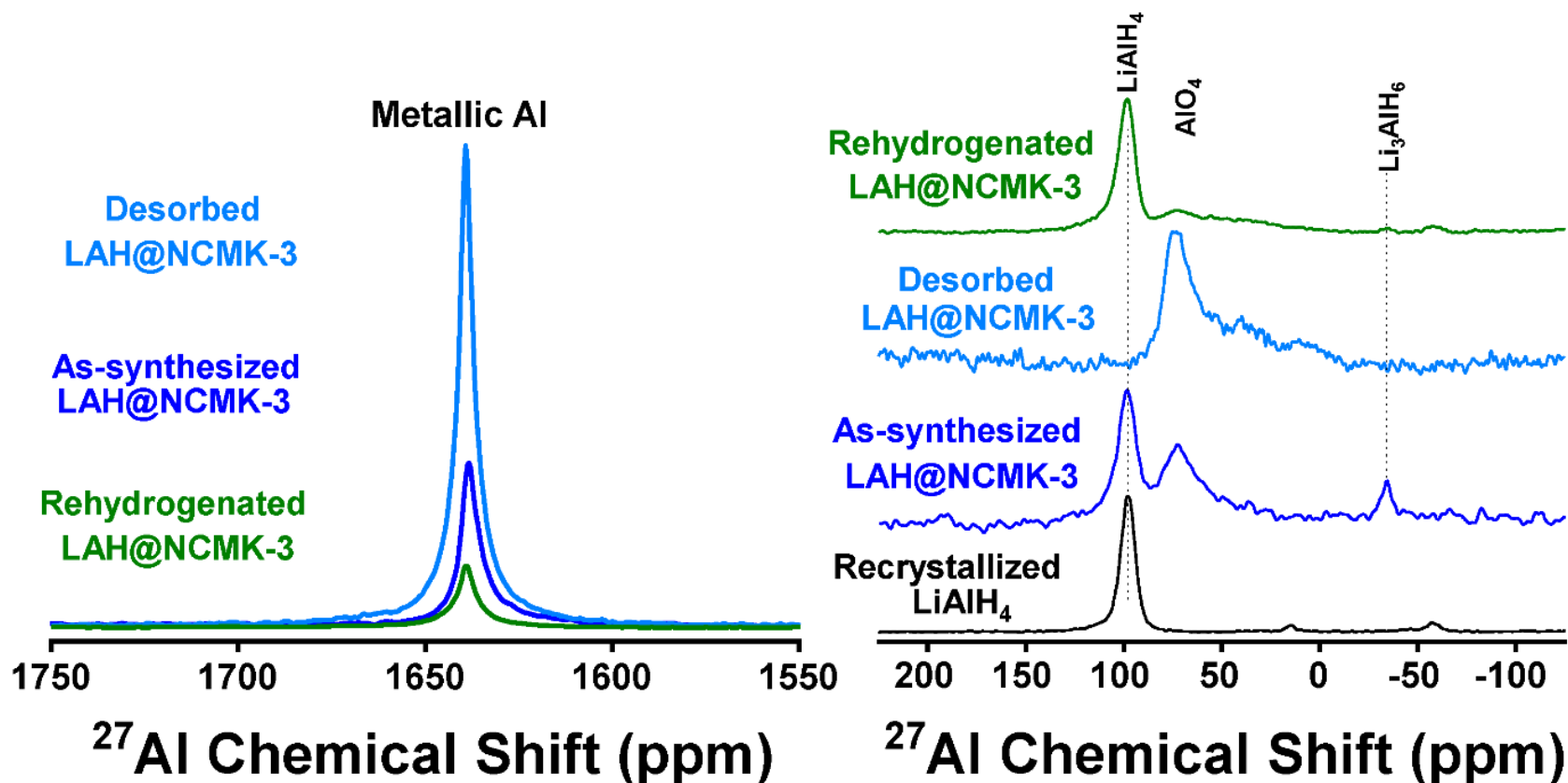
# Hydrogen release from nanoconfined $\text{LiAlH}_4$



- ⇒ The nanoconfined materials display fast kinetics of hydrogen release, and the volatiles are mostly composed of hydrogen gas and trace amounts of diethylether
- ⇒  $^{27}\text{Al}$  MAS NMR indicate that upon desorption the  $\text{LiAlH}_4\text{@NCMK-3}$  and the  $\text{LiAlH}_4\text{@CMK-3}$  samples form  $\text{LiH}$  and  $\text{Al}$  bypassing the stable  $\text{Li}_3\text{AlH}_6$  phase.



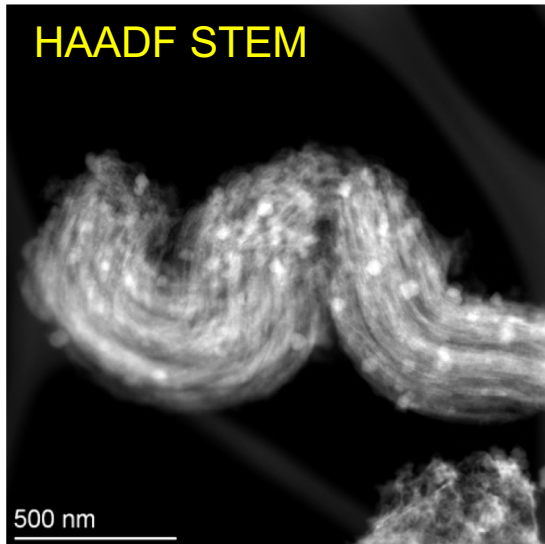
# Nitrogen doping enables partial reversibility in nano-LiAlH<sub>4</sub>



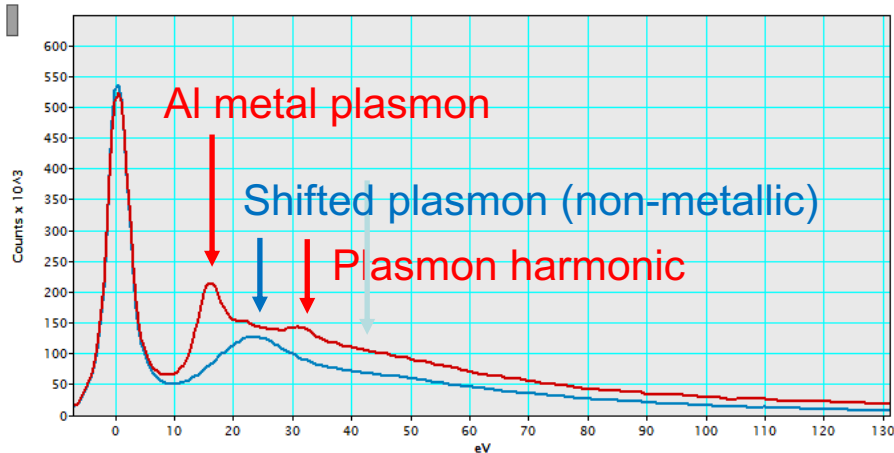
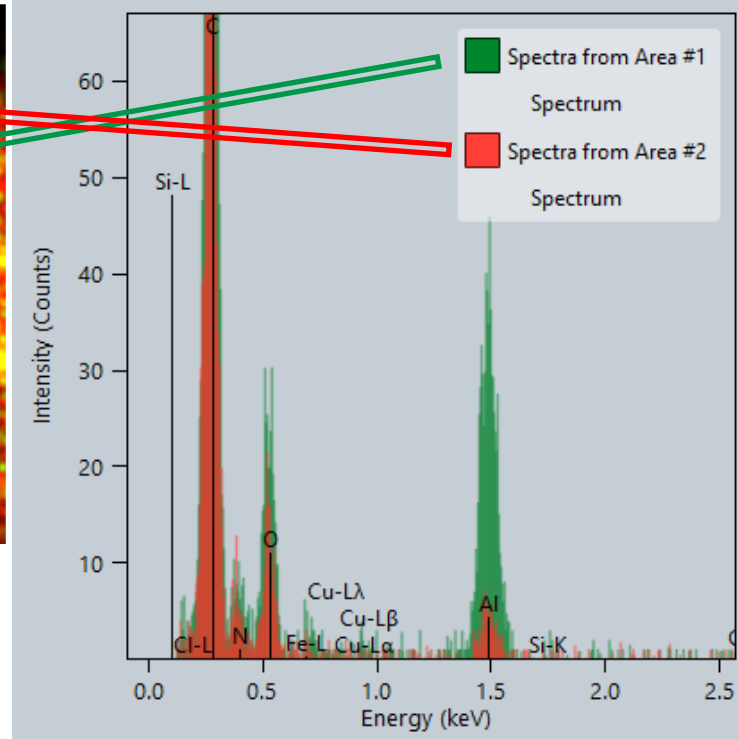
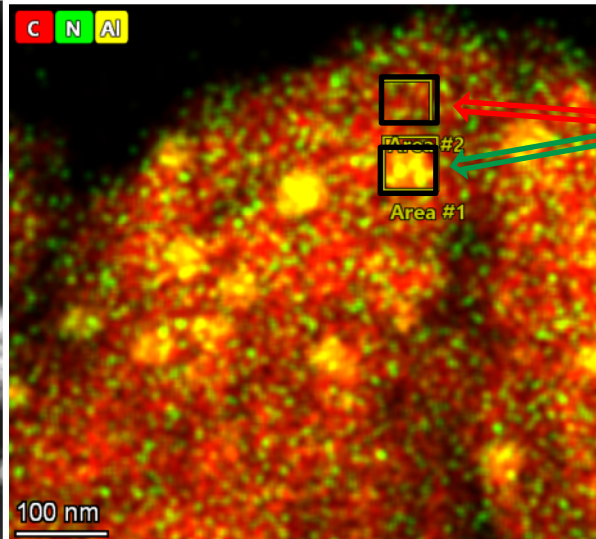
- ⇒ The MAS NMR results indicate LiAlH<sub>4</sub> decomposes at a relatively low temperature
- ⇒ The conditions for rehydrogenation are 1000 bar hydrogen pressure and 50 ° C
- ⇒ Only lithium alanate confined in N-doped CMK-3 shows partial reversibility

# TEM and EDS measurements

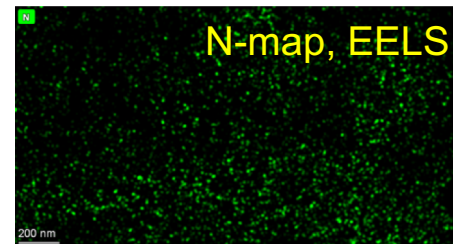
HAADF STEM



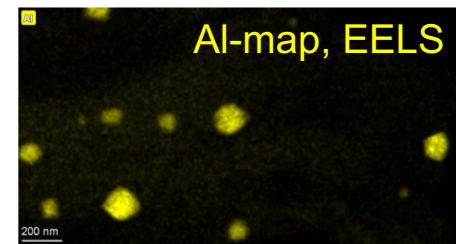
C N Al



Area 1  
Area 2



N-map, EELS

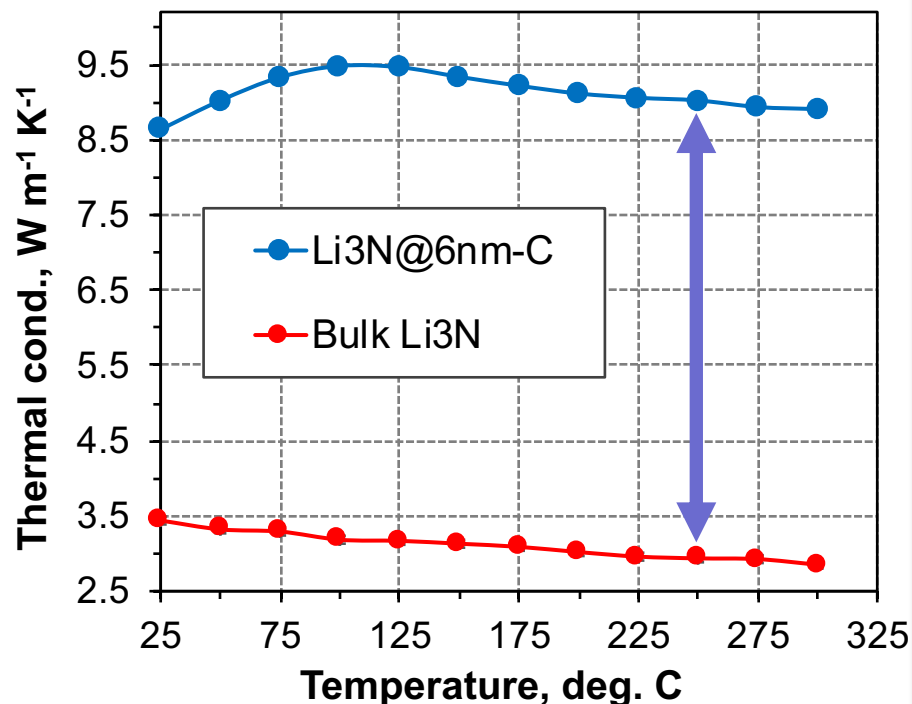


Al-map, EELS

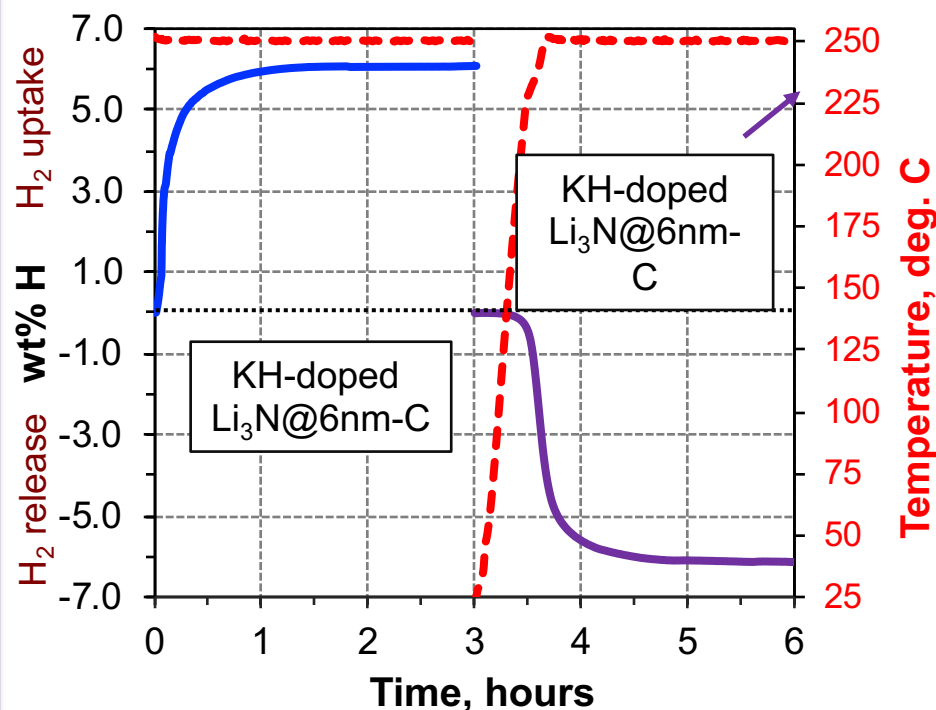
- ⇒ STEM images of rehydrogenated  $\text{LAIH}_4@\text{NCMK-3}$  showing the distribution of Al species
- ⇒ EELS spectra and maps confirm the presence of metallic Al (plasmon peak at 15 eV and the harmonic that occurs at  $2 \times 15 = 30$  eV), as well as alanate particles (plasmon peak at 24 eV).

# Enhanced thermal conductivity of $\text{Li}_3\text{N}@6\text{nm}$ -Carbon

## Thermal conductivity

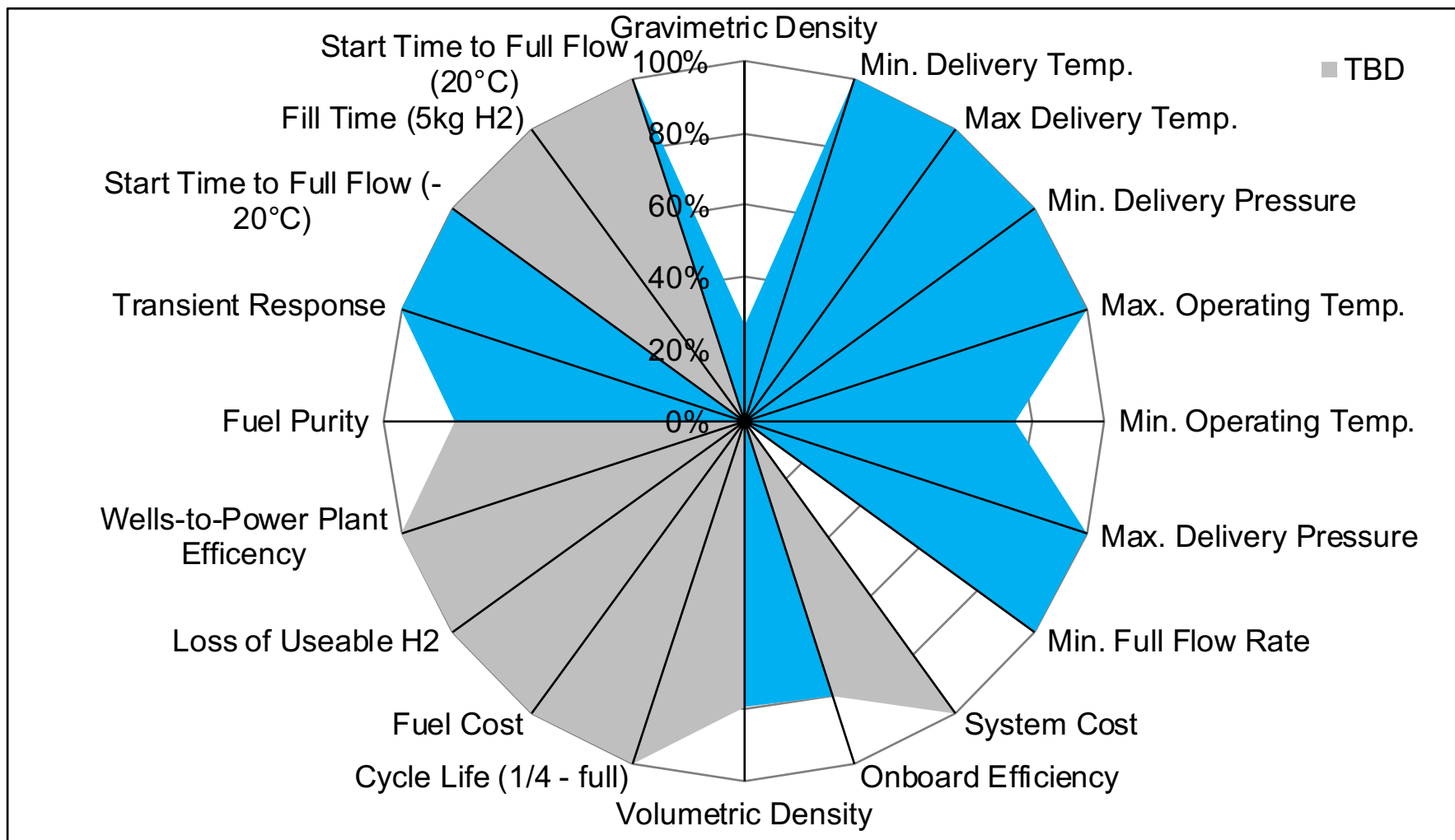


## Sieverts $\text{H}_2$ uptake and release



- Thermal conductivity of nanoconfined KH-6nm- $\text{Li}_3\text{N}@$ Carbon material is about 2.9-3.2 times higher compared to that of bulk  $\text{Li}_3\text{N}$
- The material can be reversibly cycled at 250 °C and 10.5 MPa  $\text{H}_2$

# Systems analysis on Li<sub>3</sub>N@6nm-Carbon



⇒ Finite element analysis reveals that several nanoscale metal amide/nitride materials are closer to meeting the DOE targets compared to bulk materials



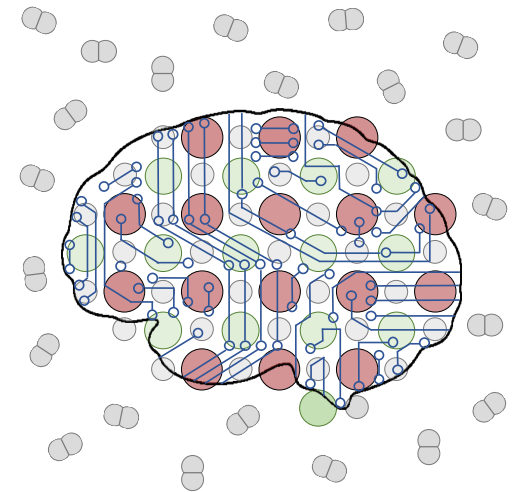
## Focus Area 2.F Development of machine-learning to discover new metal hydrides

*Decades of research on metal hydrides has failed to identify any that meet all DOE targets. Are we missing something?*

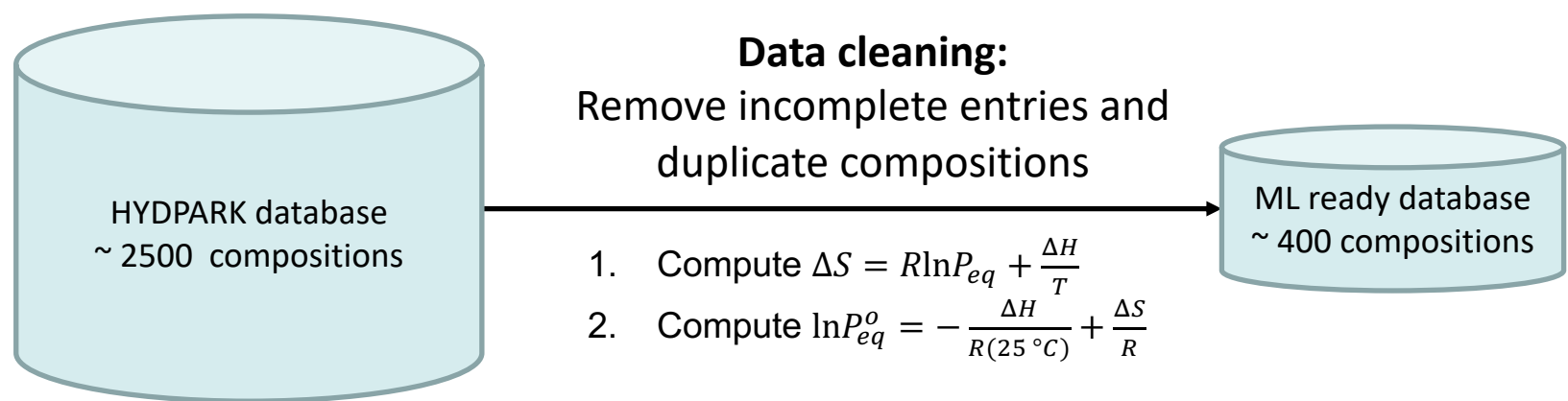
**Research Question:** Can machine learning (ML) yield physics-based insight to facilitate the design of novel metal hydrides exhibiting targeted thermodynamic properties ?

### Approach:

1. Train an ML model to predict the equilibrium plateau pressure,  $P_{eq}$ , of a metal hydride
2. Utilize the ML model's *interpretability* to understand the underlying structure-property relationships from which  $P_{eq}$  can be predicted
3. Apply these structure-property relationships to *a priori* identify known intermetallic compositions with unknown hydrides *and* are predicted to exhibit a desired  $P_{eq}$



The experimental HYDPARK database contains alloy compositions and the thermodynamics of their hydriding reactions such as  $\Delta H$ ,  $\{P_{eq}, T\}$ , and H wt. %



Comp.	$\Delta H$	$P_{eq}$	$T$	...
LaNi <sub>5</sub>				
...				
Er <sub>6</sub> Fe <sub>23</sub>				
...				
...				

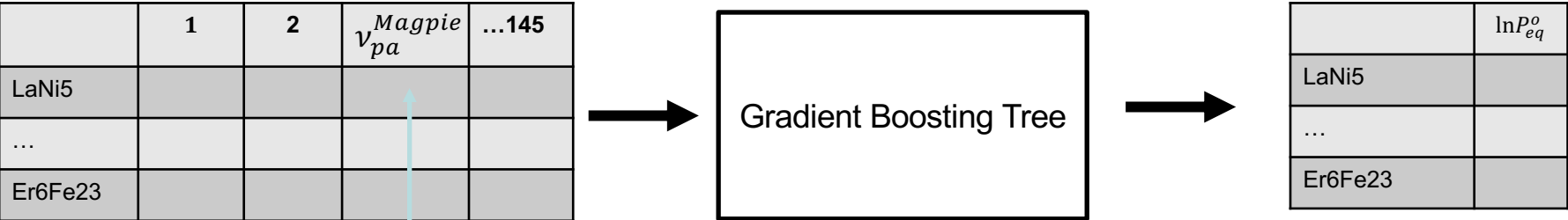
Comp.	$\Delta H$	$P_{eq}$	$T$	...	$\ln P_{eq}^o$
LaNi <sub>5</sub>					
...					
Er <sub>6</sub> Fe <sub>23</sub>					

# We created input features and chose an ML technique that promotes interpretability of the trained model to aid subsequent efforts in rational materials design

**Features:** each composition (a string) is mapped to a 145 dimensional vector computed from elemental properties using the Magpie code\*

**Model:** Gradient Boosting Trees are interpretable, i.e. they rank how important each feature is to the property prediction

**Prediction:**  $\ln P_{eq}^o$



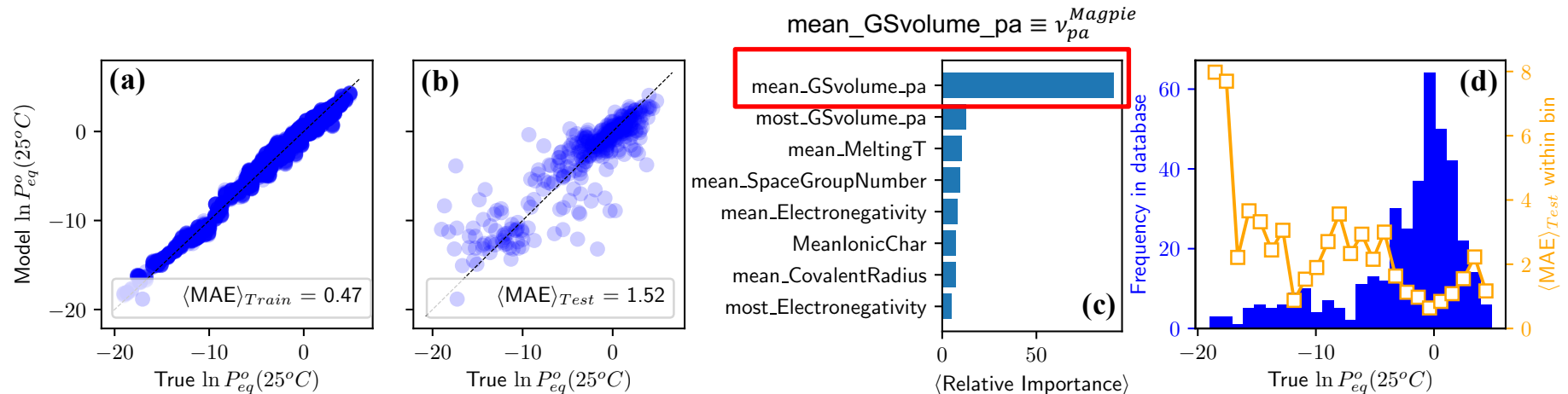
\* Developed by Wolverton and coworkers

**An example Magpie descriptor:**

$$v_{pa}^{Magpie} = \sum_i x_i v_i$$

$x_i \equiv$  composition fraction of element  $i$   
 $v_i \equiv$  ground state volume per atom of elemental solid  $i$

# ML model can predict $\ln P_{eq}^o$ with acceptable accuracy using input features derived from only the intermetallic composition



(a), (b) Model validation (test) error as quantified by the mean absolute error (MAE)

(c)  $\text{mean\_GSvolume\_pa}$  ( $v_{pa}^{Magpie}$ ) = Mean ground state volume of the unit cell (approximates volume/atom in the crystal) is the most important Magpie feature

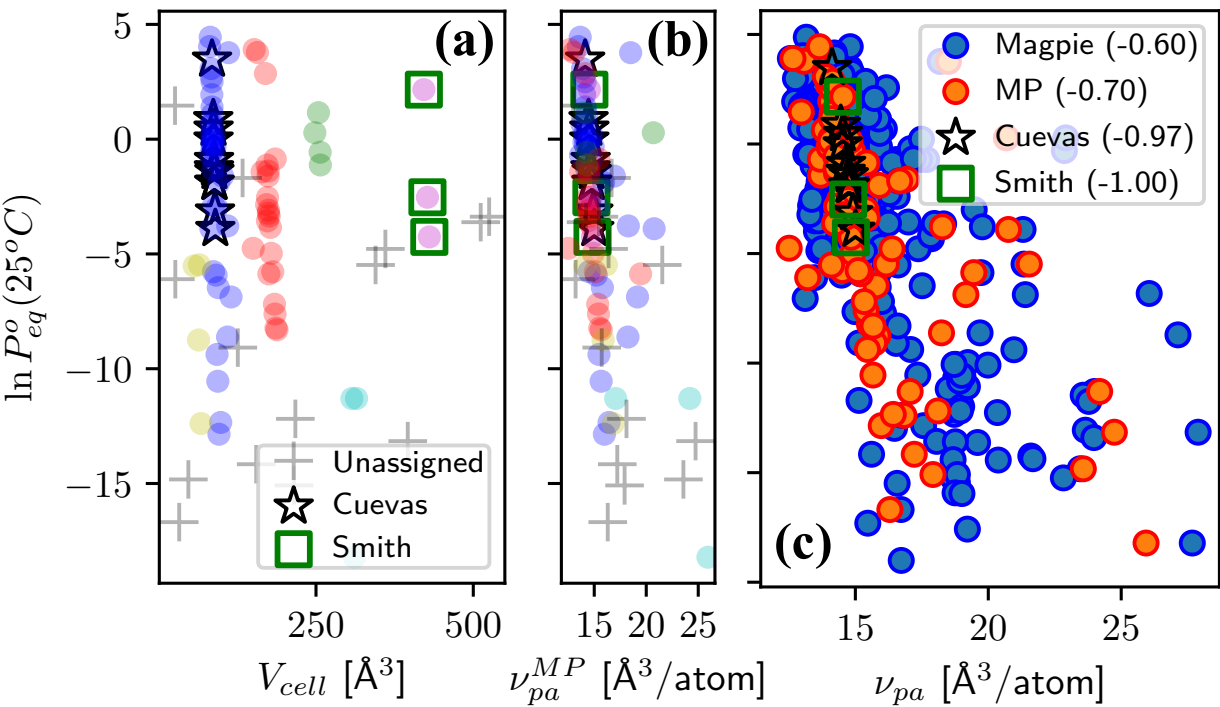
(d) Materials poorly predicted by the model are due to a large imbalance in the distribution of  $\ln P_{eq}^o$

Our data-driven approach reveals that the  $\nu_{pa}: \ln P_{eq}^o$  structure:property relationship is valid for a wide range of metal substitutions and intermetallic classes

1. Compute the structurally specific volume per atom for ~ 70 available structures in the Materials Project (MP) via:

$$V_{cell} \equiv \text{Volume of the intermetallic lattice computed in MP}$$
$$\nu_{pa}^{MP} = V_{cell}/n_{atoms}$$

2. Investigate equilibrium pressure as a function of  $\nu_{pa}^{MP}$  and  $\nu_{pa}^{MP}$ :



Cuevas et al. noted the dependence of  $\ln P_{eq}^o$  on  $V_{cell}$  in  $\text{LaNi}_5$  substitutions

Smith et al. noted the same trend for  $\text{R}_6\text{Fe}_{23}$  [R=Ho,Er,Lu] substitutions



# Utilize this structure-property relationship and DFT validation to propose a novel hydride of a known intermetallic for high-pressure H<sub>2</sub> storage applications

- Known intermetallic compound
- Hydriding properties have been reported
- Would be one of the least stable of all known experimentally reported hydrides

DFT computed properties of the *forward* (hydriding) reaction

	$\nu_{pa}$	$\Delta H$	$E_f$	$\Delta E_{def}$	$\Delta E_H$	$V/V_0$
→ UNi <sub>5</sub>	13.17	-0.60	-285	65.2	-65.8	1.278
CeNi <sub>5</sub>	13.76	-20.5	-353	49.3	-69.8	1.266
LaNi <sub>5</sub>	14.38	-36.1	-224	44.3	-80.5	1.256

Why does hydride stability tend to increase ( $\ln P_{eq}^o$  decrease) with increasing  $\nu_{pa}$ ?

1.  $\Delta E_{def}$  decreases and with it the volume expansion required for hydriding decreases  
 $\Delta E_{def}$  = energy penalty to deform lattice to accommodate H absorption (kJ/molH<sub>2</sub>)
2.  $\Delta E_H$  [kJ/molH<sub>2</sub>] (binding energy of H) tends to become more favorable
3. Together, these two effects lead to a decrease in  $\Delta H$  [kJ/mol H<sub>2</sub>], indicative of a more stable hydride

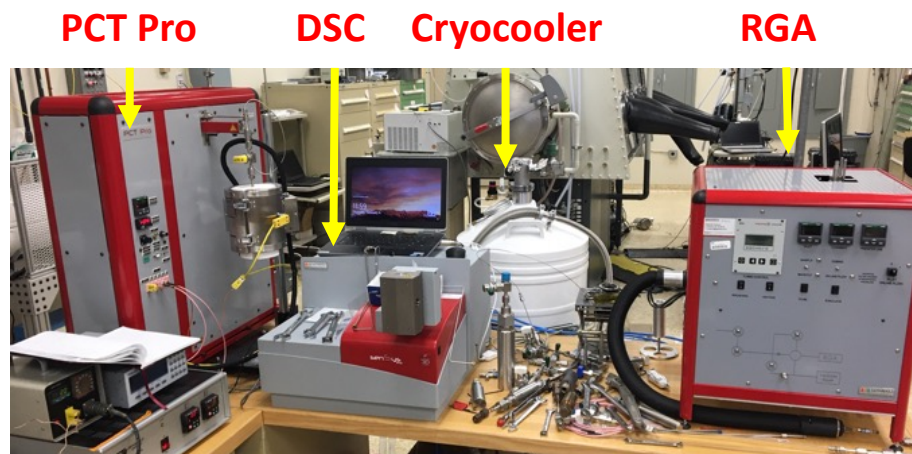
# State-of-the-art PCT with high-pressure calorimeter installed at SNL

## PCT Pro instrument

- High-accuracy pressure transducers
- Rated up to 200 bar gas pressure and 773 K
- Designed for measurements of H<sub>2</sub> and CH<sub>4</sub> uptake
- Wide range of dosing volumes

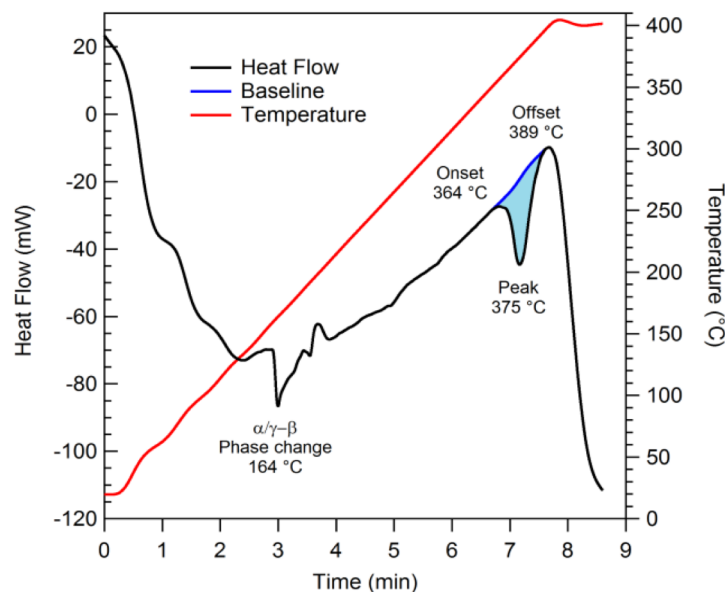
## Differential scanning calorimeter (DSC)

- SensysEvo instrument from Setaram interfaced through Swagelok connections to the PCTPro
- High-pressure DSC sample holder
  - Rated up to 431 bar gas pressure and 873 K



## Measured melting point of Mg(BH<sub>4</sub>)<sub>2</sub> under high-pressure H<sub>2</sub>

- ⇒ The observed heat flow reveals a phase change from the α and γ phases to the high-temperature β phase at ~164 °C.
- ⇒ A second endothermic peak with a temperature onset at 368 °C and a maximum at 375 °C is assigned to melting of magnesium borohydride just before thermal decomposition
- ⇒ Integrating the heat flow of the 375 °C peak yields an enthalpy 1.2 kJ·mol<sup>-1</sup>, which indicates a physical phase change process rather than a chemical reaction.



# HyMARC currently collaborates with Phase 2 Seedling Projects and facilitating their research on metal hydrides

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The HyMARC team assists individual projects with:

- A designated HyMARC point-of-contact
- Technical expertise concerning specific scientific problems
- Access to HyMARC capabilities
- ***Magnesium Boride Etherates as Hydrogen Storage Materials*** (U. Hawaii, G. Severa, Lead)
  - 18 modified  $\text{MgB}_2$  samples for ultrahigh-P hydrogenation
  - 12 modified  $\text{MgB}_2$  samples for XAS at the ALS
- ***Electrolyte Assisted Hydrogen Storage Reactions*** (LiOx Power, J. Vajo, Lead)
  - 4 samples for ultrahigh-P hydrogenation
- ***ALD Synthesis of Novel Nanostructured Metal Borohydrides*** (NREL, S. Christensen, Lead)
  - 4 samples for ultrahigh-P hydrogenation



# HyMARC-NSF seedling projects

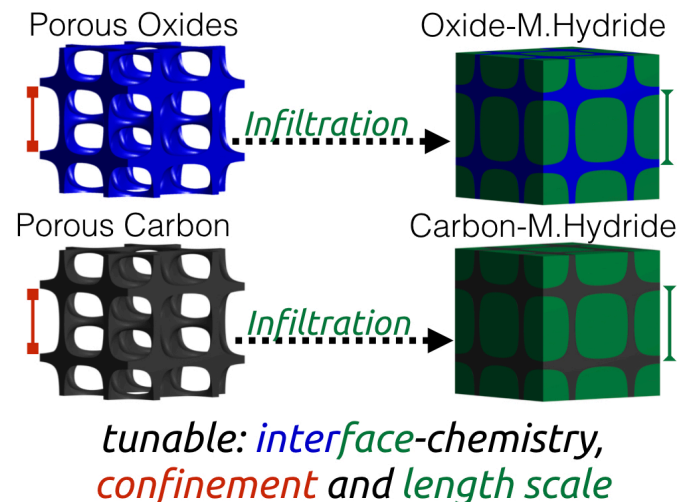
## FY19 SSMC-EMN Supplemental Funding Opportunity

### Tunable Isomorphic Architectures for Hydrogen Storage

Prof. Morgan Stefik, Univ. South Carolina

[stefik@mailbox.sc.edu](mailto:stefik@mailbox.sc.edu)

- Visit by graduate student Eric Williams Nov., 2019
- Synthesis of narrow-pore carbons



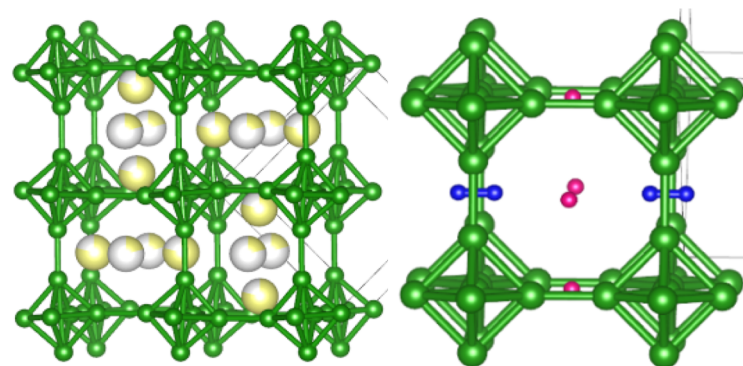
### Transition Metal-Free Borides for Hydrogen Storage

FY19 SSMC-EMN Supplemental Funding Opportunity

Prof. Viktor Poltavets, Univ. New Orleans

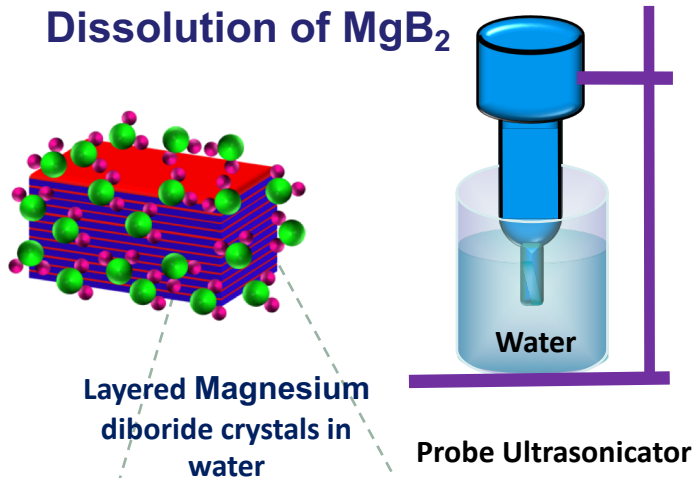
[vpoltave@uno.edu](mailto:vpoltave@uno.edu)

- Visit by grad. student Roshni Bhuvan Oct-Nov 2019
- High-pressure rehydrogenation of doped-MgB<sub>2</sub>

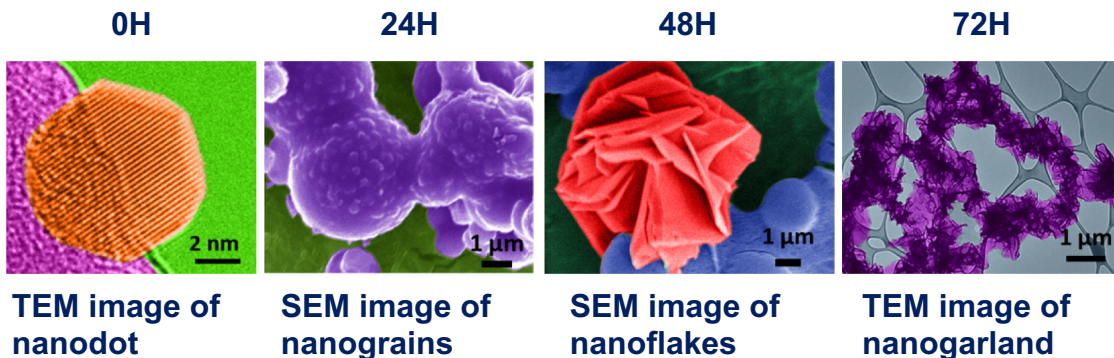


# Mg-B nanosheets: Collaboration with IIT Gandhinagar (India)

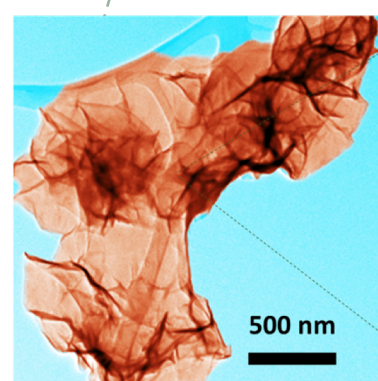
## Dissolution of $\text{MgB}_2$



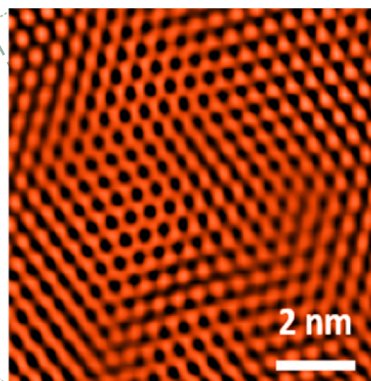
## Recrystallization on aging



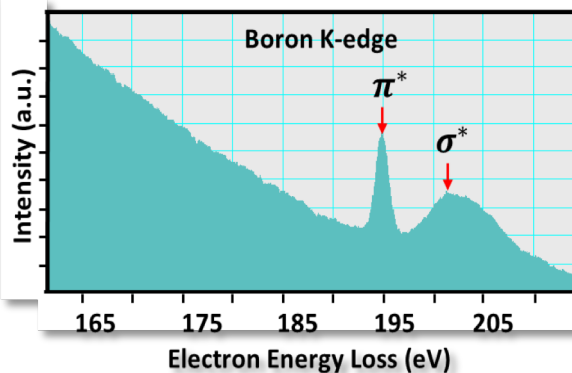
## Characterization of Mg-B nanostructures



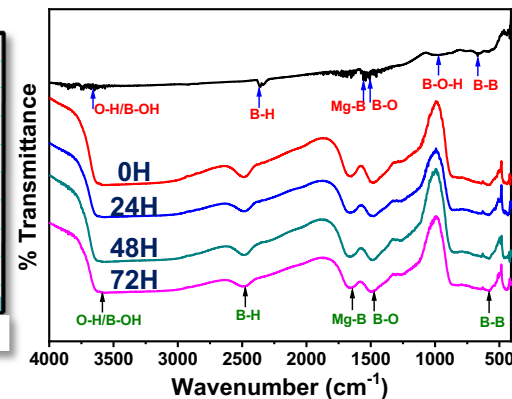
TEM image of a nanosheet



Hexagonal honeycomb network of boron atoms



Boron EELS obtained from a nanosheet

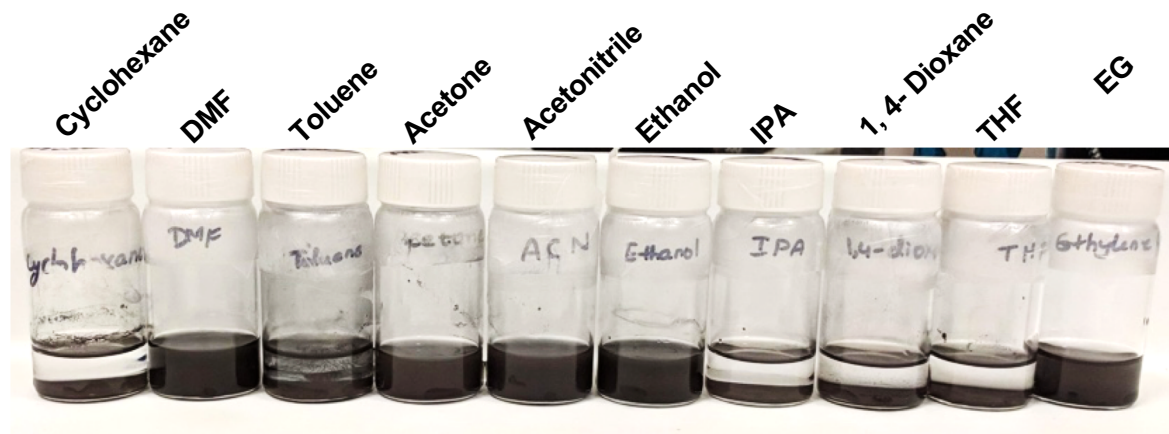
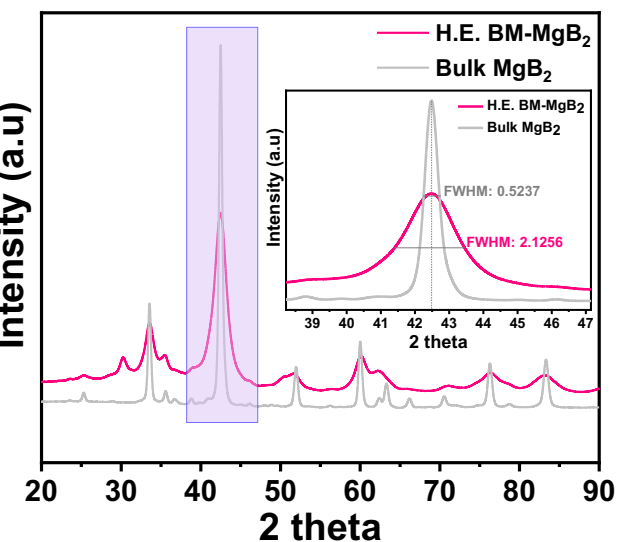
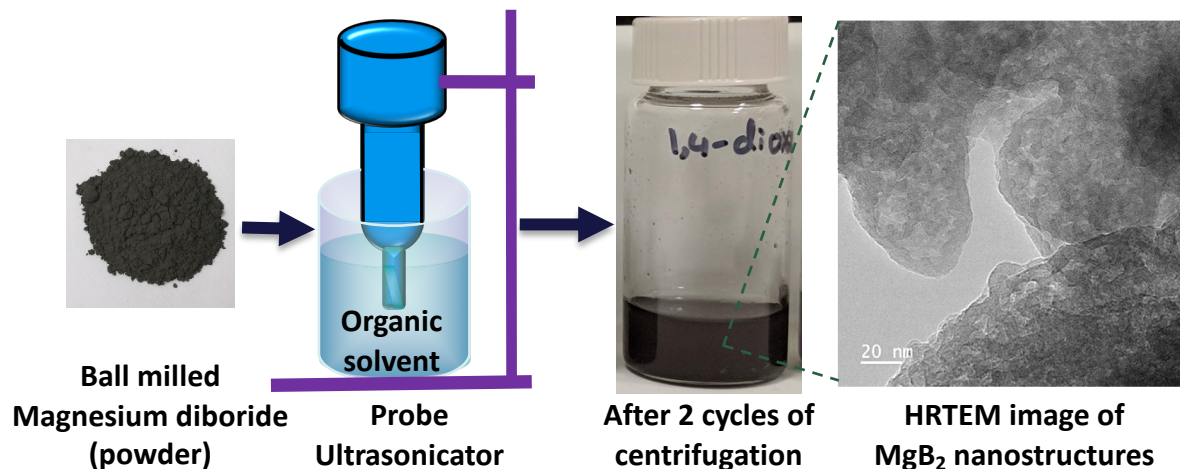
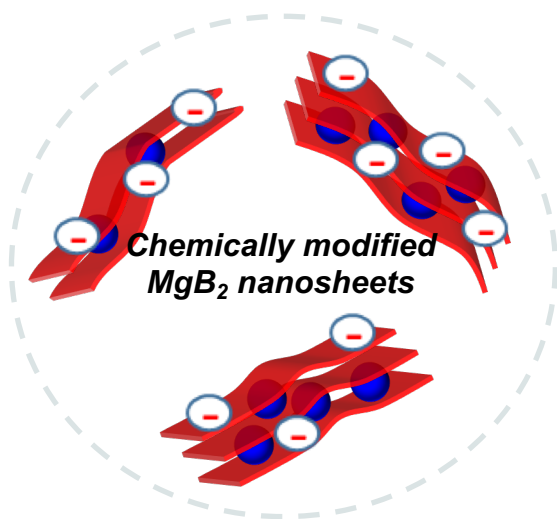


FTIR analysis of nanostructures

⇒ Examining  $\text{MgB}_2$  nanosheets to see if they have increased reactivity in hydrogen storage reactions



# Exfoliation of $\text{MgB}_2$ in non-aqueous solvents



*Matching surface energy of  $\text{MgB}_2$  and its polar and dispersive component ratios*

*DMF, ACN, ACETONE, ETHANOL, and EG produce  $\text{MgB}_2$  nanostructures*

⇒ The ability to create  $\text{MgB}_2$  nanostructures depends on the nature of the solvent and surface energy

# Collaboration and Coordination

- Timmy Ramirez (Oak Ridge National Lab, USA) : VISION, inelastic neutron scattering
- John J. Vajo, Jason Graetz (HRL Labs, USA): Electrolyte-promoted H<sub>2</sub> storage reactions
- Craig Jensen, Godwin Severa (University of Hawaii): borohydrides for hydrogen storage
- Karl Gross (H<sub>2</sub> Technology Consulting, USA): PCT measurements on metal hydrides
- Morgan Stefik, (University of South Carolina, USA): carbon hosts for nanoconfinement
- Viktor Balema, Vitalij Pecharskij (AMES Lab, USA): metal hydrides, mechanochemistry
- Dhanesh Chandra (University of Nevada, Reno, USA): CALPHAD and phase diagrams
- Dallas Trinkle (UIUC, USA): Predicting hydrogen diffusion in metal hydrides
- Martin Dornheim (Helmholtz-Zentrum Hamburg, Germany): metal hydride composites
- Sanliang Ling (University of Nottingham): DFT calculations and machine learning
- Bettina Lotsch (MPI Festkoerperforschung, Germany): Bypyridine-functionalized hosts
- Torben Jensen (Aarhus University, Denmark): metal borohydrides for hydrogen storage
- Martin Sahlberg (Uppsala University, Sweden): high-entropy alloys for H<sub>2</sub> storage
- David Fairen-Jimenez (University of Cambridge, UK): synthesis of hydride/MOF composites
- Harini Gunda, Kabeer Jasuja (IIT Gandhinagar, India): metal boride nanosheets for H<sub>2</sub> storage
- Shin-ichi Orimo (Tohoku University, Japan): characterization of metal *closo*-borates
- Eun Seon Cho (KAIST, South Korea): strain-induced destabilization of metal hydrides

# Publications and Presentations

## Selected Papers:

- J.L. White, N.A. Strange, J.D. Sugar, J.L. Snider, A. Schneemann, A.S. Lipton, M.F. Toney, M.D. Allendorf, V. Stavila, "[Melting of Magnesium Borohydride under High Hydrogen Pressure: Thermodynamic Stability and Effects of Nanoconfinement](#)" *Chemistry of Materials*, accepted (2020)
- A. Schneemann, L.F. Wan, A.S. Lipton, Y.-S. Liu, J.L. Snider, A.A. Baker, J.D. Sugar, C.D. Spataru, J. Guo, A.S. Autrey, M. Jørgensen, T.R. Jensen, B.C. Wood, M.D. Allendorf, and V. Stavila, "[Limit of nanoconfinement? 'Molecular' magnesium borohydride captured in a bipyridine-functionalized metal-organic framework](#)," submitted to *ACS Nano* (2020)
- B.C. Wood, T.W. Heo, S. Kang, S. Li, and L.F. Wan, "[Beyond idealized models of nanoscale metal hydrides for hydrogen storage](#)" *Ind. Eng. Chem. Res.*, **13**, 5786–5796 (2020) [invited article].
- S. Jeong, T.W. Heo, J. Oktawiec, R. Shi, S. Kang, J.L. White, A. Schneemann, E.W. Zaia, L.F. Wan, K.G. Ray, Y.-S. Liu, V. Stavila, J. Guo, J.R. Long, B.C. Wood, and J.J. Urban, "[A Mechanistic Analysis of Phase Evolution and Hydrogen Storage Behavior in Nanocrystalline Mg\(BH<sub>4</sub>\)<sub>2</sub> within Reduced Graphene Oxide](#)" *ACS Nano*, **14**, 1745–1756 (2020).
- J.L. White, A.A. Baker, M.A. Marcus, J.L. Snider, T. C. Wang, J.R.I. Lee, D.A.L. Kilcoyne, M.D. Allendorf, V. Stavila, FEI Gabaly, "[The Inside-Outs of Metal Hydride Dehydrogenation: Imaging the Phase Evolution of the Li-N-H Hydrogen Storage System](#)" *Adv. Mater. Interfaces*, **7**, 1901905 (2020).
- T.W. Heo and B.C. Wood, "[On thermodynamic and kinetic mechanisms for stabilizing surface solid solutions](#)" *ACS Appl. Mater. Interf.* **11**, 48487 (2019).
- T.W. Heo, K.B. Colas, A.T. Motta, and L.-Q. Chen, "[A phase-field model for hydride formation in polycrystalline metals: Application to  \$\delta\$ -hydride in zirconium alloys](#)," *Acta Mater.* **181**, 262 (2019).
- Y.-S. Liu, L.E. Klebanoff, P. Wijeratne, D.F. Cowgill, V. Stavila, T.W. Heo, S. Kang, A.A. Baker, J.R.I. Lee, K.G. Ray, J.D. Sugar, and B.C. Wood, "[Investigating possible kinetic limitations to MgB<sub>2</sub> hydrogenation](#)", *Int. J. Hydrogen Energy* **44**, 31239 (2019).

## Presentations:

37 presentations (3 keynote and 15 invited) at national and International conferences and symposia.

**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**



***Enabling **twice the energy density** for onboard  $H_2$  storage***