
HyMARC: A Consortium for Advancing Hydrogen Storage Materials

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Overall Objectives

- Accelerate discovery of breakthrough storage materials by developing foundational understanding of phenomena governing thermodynamics and kinetics.
- Develop community tools and capabilities to enable materials discovery, including computational models and databases, new characterization tools and methods, and tailorable synthetic platforms.
- Provide technical direction to the Hydrogen Materials Advanced Research Consortium (HyMARC) via leadership of Task 1 (Thermodynamics), Task 3 (Gas Surface Interactions), and Task 5 (Additives).
- Provide gas sorption and other property data needed to develop thermodynamic models of sorbents and metal hydrides, including the effects of ultrahigh hydrogen pressure.
- Identify the structure, composition, and reactivity of gas-surface and solid-solid hydride surfaces contributing to rate-limiting desorption and uptake.
- Synthesize metal hydrides and sorbents in a variety of formats (e.g., bulk powders, thin

films, nanostructures) and develop in situ techniques for their characterization.

- Apply Sandia National Laboratories (SNL) multiscale codes to discover new materials and new mechanisms of storing hydrogen, and provide input for database development.
- Elucidate the role of additives in improving hydrogen uptake and release from materials.

Fiscal Year (FY) 2018 Objectives

- Perform sensitivity analysis of local binding and second-sphere effects.
- Rank improvement strategies for sorbents and metal hydrides.
- Develop a modeling formalism for amorphous phases and defects.
- Parameterize integrated kinetic model for representative B-N-Al hydrides.
- Compute sorbent isotherms from quantum Monte Carlo data for metal-organic frameworks (MOFs).
- Publicly release codes, databases, synthetic protocols, and characterization methodologies optimized for storage materials.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan¹:

- (O) Lack of Understanding of Hydrogen Physisorption and Chemisorption
- (A) System Weight and Volume
- (E) Charging/Discharging Rates
- (F) Cost, Efficiency, Durability.

¹ <https://www.energy.gov/eere/fuelcells/downloads/fuel-cell-technologies-office-multi-year-research-development-and-22>

Technical Targets

The goal of this project is to develop foundational understanding of phenomena governing thermodynamics and kinetics of hydrogen release and uptake in all classes of hydrogen storage materials. Insights gained from these studies will be applied toward the design and synthesis of hydrogen storage materials that meet the following DOE 2020 hydrogen storage targets:

- Cost: \$10/kWh net
- Specific energy: 1.8 kWh/kg
- Energy density: 1.3 kWh/L.

FY 2018 Accomplishments

- Predicted and measured thermodynamic data for $\text{Mg}(\text{BH}_4)_2$ needed to establish a validated phase diagram for this storage material.
- Determined that B-B bond activation, not H_2 bond breaking, is the rate-limiting step in the hydrogenation of MgB_2 .
- Determined the enthalpy and entropy of hydrogen desorption from bulk $\text{Mg}(\text{BH}_4)_2$, crucial data for which accurate values were lacking in the literature.
- Created a new melt-infiltration method for $\text{Mg}(\text{BH}_4)_2$ incorporation into porous hosts for synthesizing nanoscale hydrogen storage materials.
- Discovered that some MOF sorbents are not completely stable under high hydrogen pressure or upon repeated high-pressure hydrogen cycling.
- Performed the first in situ characterization of the surface chemistry of $\text{Mg}(\text{BH}_4)_2$ using synchrotron methods and low-energy ion scattering (a unique HyMARC capability), showing that the surface composition evolves in time.
- Determined the melting temperature of $\text{Mg}(\text{BH}_4)_2$ under 1,000-bar hydrogen pressure using a unique high-pressure reactor system at SNL.
- Measured low- and high-pressure hydrogen isotherms for validating computational models of hydrogen uptake by nanoporous sorbents.

- Initiated a comprehensive force-field development effort for Mg-B-H intermediates.
- Developed validated molecular dynamics models of hydrogen diffusion in magnesium hydride (MgH_2).
- Developed a new methodology for simulating nucleation kinetics of complex metal hydrides.
- Published a major review on nanoscale metal hydrides and a perspective article concerning strategies for developing new sorbent materials.

INTRODUCTION

Storage of hydrogen onboard vehicles is one of the critical technologies needed to create hydrogen-fueled transportation systems that can improve energy efficiency and resiliency, reduce oil dependency, and promote energy independence. Stakeholders in developing hydrogen infrastructure (e.g., state governments, automotive original equipment manufacturers, station providers, and industrial gas suppliers) are currently focused on high-pressure storage at 350 bar and 700 bar, in part because no viable solid-phase storage material has emerged. Early-stage research to develop foundational understanding of solid-state storage materials, including novel sorbents and high-density hydrides, is of high importance because of their unique potential to meet all DOE Fuel Cell Technologies Office targets and deliver hydrogen at lower storage pressures and higher onboard densities. However, existing materials suffer from thermodynamic and kinetic limitations that prevent their application as practical hydrogen storage media.

SNL's overall objectives and responsibilities within HyMARC are to (1) provide technical leadership to the consortium at the director level, as well as through leadership of Task 1 (Thermodynamics), Task 3 (Gas Surface Interactions), and Task 5 (Additives); (2) provide gas sorption and other property data required to develop and validate thermodynamic models of sorbents and metal hydride storage materials, including the effects of 350 bar and 700 bar hydrogen delivery pressures, serving as a resource for the consortium; (3) identify the structure, composition, and reactivity of gas surface and solid-solid hydride surfaces contributing to rate-limiting desorption and uptake; (4) provide metal hydrides and MOF sorbents in a variety of formats tailored for specific consortium tasks; (5) develop sample preparation methods and experimental protocols to enable facile use of the new characterization probes employed by HyMARC; (6) apply SNL multiscale codes to discover diffusion pathways and mechanisms of storage materials; and (7) elucidate the role of additives in promoting hydrogen storage reactions.

APPROACH

HyMARC seeks to address critical gaps in the science of hydrogen storage by leveraging recent advances in predictive multiscale modeling, high-resolution in situ characterization, and novel material synthesis techniques. By focusing on the underlying thermodynamic and kinetic limitations of storage materials, we will generate foundational understanding that will accelerate the development of all types of advanced storage materials, including sorbents, metal hydrides, and liquid carriers.

RESULTS

Substantial progress was made on each of the five tasks being performed at SNL, with all of the quarterly goals met on time. SNL principal investigators led the organization of task groups, helping to guide the science in collaboration with our partners, and scheduling and coordinating task team meetings involving all three HyMARC laboratory partners. Technical results include the following.

Task 1: Thermodynamics

SNL's effort to elucidate the factors contributing to the thermodynamics of hydrogen uptake and release by sorbents and metal hydrides provided new data and contributed to the foundational understanding of these materials.

Key results for metal hydrides: The thermodynamics of metal hydrides are a major focus of HyMARC, as these determine the conditions required to release hydrogen and recharge the storage material. Magnesium borohydride ($\text{Mg}(\text{BH}_4)_2$) stands out among the many known metal hydrides as a material with the gravimetric and volumetric capacity required to meet the DOE technical targets. However, its thermodynamic properties, including enthalpy and entropy of hydrogen desorption and the stability of its decomposition products, are poorly understood. Through experimental measurements in SNL's ultrahigh-pressure reactor, we determined for the first time that $\text{Mg}(\text{BH}_4)_2$ melts at 365°C under 1,000 bar hydrogen. We also determined that the hydrogen desorption enthalpy for the bulk material is 48 kJ/mol H_2 , indicating that its thermodynamic properties are far from optimum. These new data allowed us to develop a method to melt-infiltrate porous

materials with the hydride to create nanoparticles. Moreover, these nanoparticles begin to release hydrogen at temperatures 100°–150°C lower than the bulk, suggesting a new strategy for increasing the kinetics of hydrogen release from borohydrides. Our measurements were also used to calibrate the Mg-B-H phase diagram theoretically predicted by Lawrence Livermore National Laboratory (LLNL) (Figure 1). In this phase diagram prediction, *ab initio* molecular dynamics (AIMD) simulations were used to account for anharmonic vibrations of $B_xH_y^{n-}$ molecules. The predicted temperature-pressure conditions for phase coexistence were calibrated using the SNL pressure-composition-temperature (PCT) data. Our efforts to achieve more accurate predictions enabled us to greatly reduce the errors in the predicted reaction entropies and enthalpies. Compared with errors in these quantities of 11% and 50%, respectively, we achieved errors <3% and 12%. The validated phase diagram was used to distinguish thermodynamic products from those resulting from slow chemical kinetics.

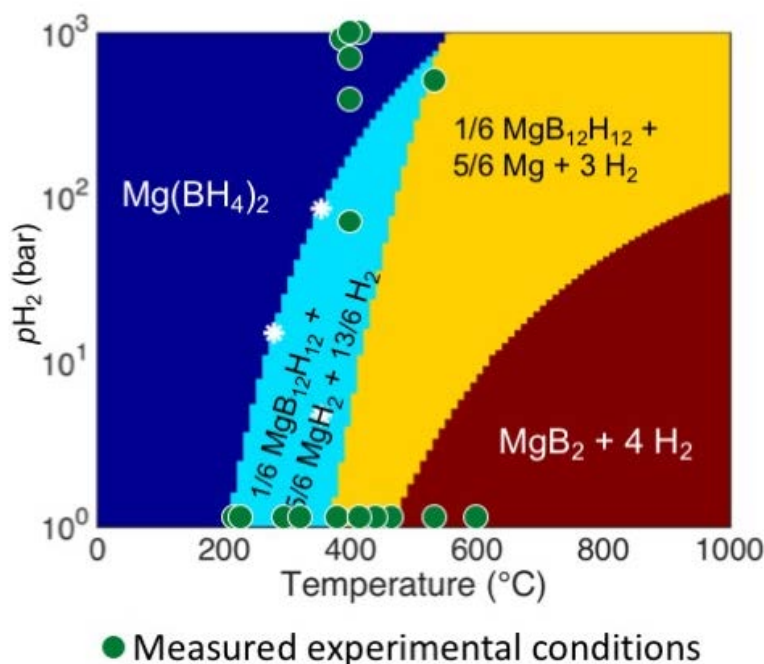


Figure 1. Comparison of Mg-B-H phase diagram, computed using density functional theory, with experimentally measured equilibrium hydrogen pressures

We also applied our computational method for calculating hydride entropies to all experimentally observed or theoretically predicted intermediate compositions and polymorphs of the Li-N-H, Na-Al-H, Li-B-H, Na-B-H, and Mg-B-H systems. An advantage of our approach is that it can separate the anharmonic and harmonic contributions to the entropy. We estimate that the former contributes up to 10 kJ/mol H_2 at 700 K, or 50% of the harmonic contributions. Consequently, we developed a new hypothesis that a “freezing” confining medium that interacts strongly with the metal hydride may suppress these anharmonic phonon modes, which could help to decouple entropic and enthalpic thermodynamic contributions.

Key results for sorbents: MOFs are a promising class of tailorable nanoporous sorbent materials that are being intensively investigated for hydrogen storage. Understanding their long-term stability under repeated cycles of low- to high-pressure hydrogen is essential for determining their long-term potential. We selected a suite of eight MOFs to compare the effects of metal ion redox activity, pore volume, and chemical structure of the organic linker groups on stability toward hydrogen cycling. The MOFs were subjected to two different

tests under the hydrogen environment: (1) extensive cycling (1,000 cycles) between 5 bar and 100 bar in hydrogen at room temperature, and (2) ultrahigh pressure (700 bar) of hydrogen at room temperature. Characterization of the MOF materials following these tests showed that most of the MOFs are stable under these conditions, with the exception of IRMOF-74-II(Mg) and IRMOF-74(Ni). IRMOF-74-II(Mg) showed ~10% loss in porosity after extensive cycling between 5 and 100 bar, and MOF-74(Ni) showed 10%–20% loss in porosity under both conditions. A detailed transmission electron microscopy study of the MOF-74(Ni) sample clearly indicates the formation of 3–5 nm nickel nanoparticles in the MOF structure. The reasons for this instability are currently under investigation.

Task 2: Kinetics of Mass Transport

We developed an automated software tool for accelerating the development and optimization of force fields for simulating the mass transport kinetics of hydrogen and other elements through storage materials. Mass transport is one of the primary phenomena affecting rates of hydrogen release and uptake by metal hydrides. Molecular dynamics methods, which assume that Newton's laws govern mass transport, are a powerful approach to simulating these processes, but they require a comprehensive force field to describe correctly the potential energy surfaces within a material. For complex molecular systems, intermolecular interactions depend on molecular species and both the spacing and relative orientation between molecules. As a result, force field development is very time consuming, as multiple parameters must be fit to thousands of target values obtained from density functional theory calculations. The parameterization tool we developed is highly automated: the only inputs required from the user are the chemical formulae of all molecules included in the simulation and files containing intermolecular interaction energies obtained from density functional theory. Each iteration of force field optimization can be completed within a matter of a few days rather than months. Using this approach, we developed a validated model for hydrogen diffusion through magnesium that accurately captures the crystalline growth of MgH_2 .

Task 3: Surface Science

Using a suite of cutting-edge characterization tools that probe the surface, near-surface, and bulk regions of a hydrogen storage material, we showed for the first time that the surface of complex metal hydrides evolves dynamically as hydrogen is desorbed. Of particular significance is our observation that oxygen-containing surface species are actively involved in the release of hydrogen from titanium-doped NaAlH_4 . Titanium is a well-known additive that enables the reversible release and uptake of hydrogen by this hydride, but despite extensive study (>2,000 papers published) the mechanism is still not firmly established. We employed two *in operando* diagnostics: low-energy ion scattering (LEIS) at SNL, which is uniquely sensitive to hydrogen on the monolayer atomic surface of a material, and the synchrotron-based ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) facility at the Advanced Light Source (at Lawrence Berkeley National Laboratory [LBNL]), which probes the surface and subsurface (0–10 nm). In addition, we used scanning transmission X-ray microscopy (STXM) to probe the distribution of chemical species within bulk particles. Data interpretation from the two X-ray tools was facilitated by computational spectroscopy at the Molecular Foundry, located at LBNL, and at LLNL. XPS chemical shifts were computed for active species involved in dehydrogenation, based on local configurations derived from AIMD simulations. Dehydrogenation kinetics were also studied using direct barrier calculations. The results demonstrate that titanium-containing surface species play no direct role in the surface desorption chemistry. Rather, they suggest that surface hydroxides may actually facilitate surface hydrogen formation and release. This represents a paradigm shift concerning the role of surface oxygen, which is unavoidable for these highly reactive materials, and is consequently influencing the way we conceive of new hydride-based storage materials.

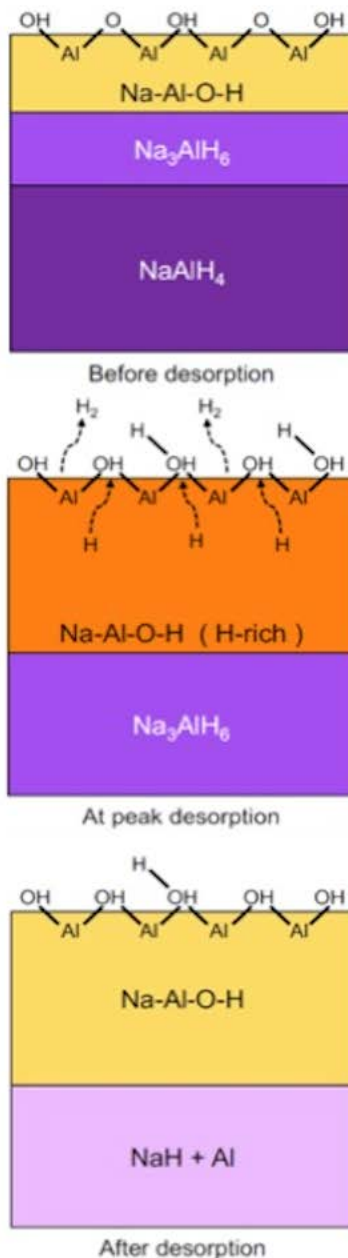


Figure 2. Schematic describing desorption of H_2 from $NaAlH_4$. During desorption, the hydrogen concentration increases in the surface oxide layer. After desorption, its concentration decreases, indicating that either H diffusion through the oxygen layer or H_2 recombination on the surface is rate-limiting.

Task 4: Solid-Solid Interfaces

We employed the Task 3 diagnostic suite to probe the uptake of hydrogen by $Mg(BH_4)_2$. Preliminary LEIS results show that we can detect hydrogen on the hydride surface. AP-XPS measurements indicate that Mg segregates to the surface during uptake and the concentration of surface boron increases during hydrogen release. Interestingly, STXM measurements at the UVSOR synchrotron in Japan show that the hydride decomposition propagates from the inside outward, contradicting the initial hypothesis (Figure 3). This behavior is similar to that found for lithium amide ($LiNH_2$), namely, that the most hydrogenated phase is present on the exterior of each particle regardless of the direction or degree of hydrogenation. These results are now being used to inform our development of models to simulate hydrogen release from borohydrides.

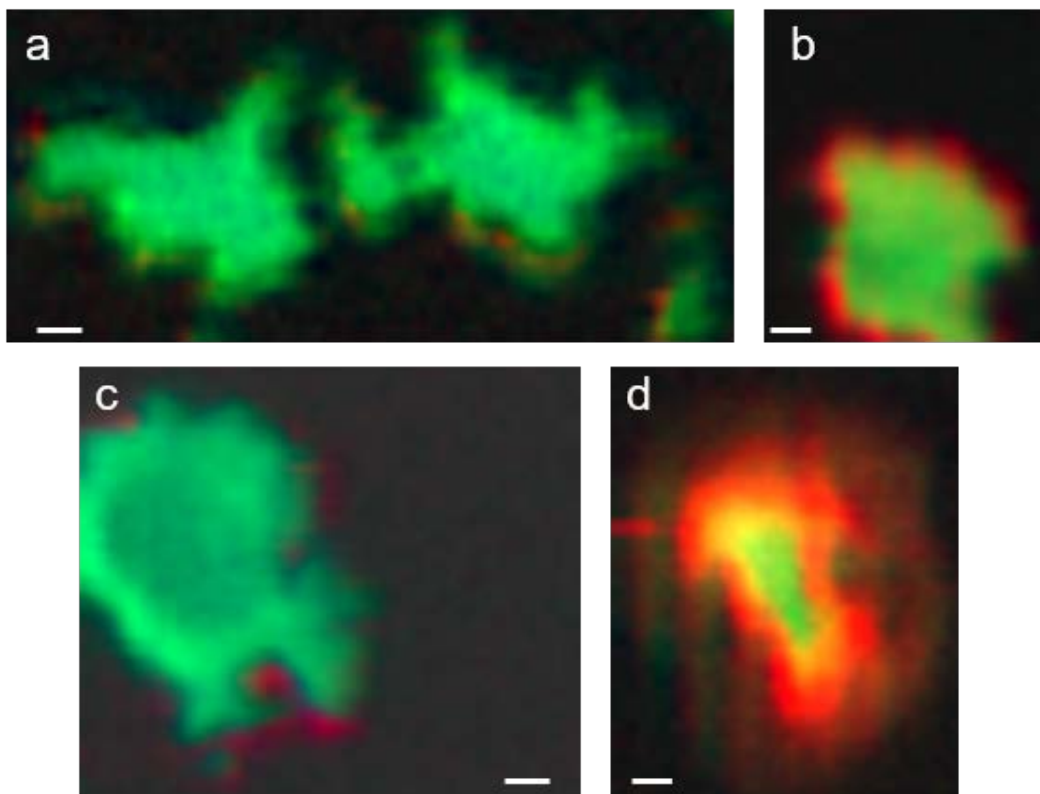


Figure 3. STXM images of samples treated at 400 °C for 72 h: (a) MgB_2 under 202 bar H_2 , (b) $\text{Mg}(\text{BH}_4)_2$ under 202 bar H_2 , (c) MgB_2 under 700 bar H_2 , (d) $\text{Mg}(\text{BH}_4)_2$ under 360 bar H_2 . Red regions correspond to $\text{Mg}(\text{BH}_4)_2$; green regions represent $\text{MgB}_{12}\text{H}_{12}$.

To understand the observed phase behavior during (de/re)hydrogenation, we formulated a computational model for complex hydrides based on advanced phase nucleation theory and involving multiple intermediates. As an initial test case, the model was parameterized by our *ab initio* thermodynamics calculations for the Mg-B-H system. We conducted a preliminary investigation of possible kinetic pathways that may lead to different types of phase microstructures. For hydrogenation of a MgB_2 particle through the $\text{MgB}_{12}\text{H}_{12}$ intermediate, we identified multiple possible phase transformation pathways by examining the phase nucleation barriers as a function of particle size and surface/interfacial energies. This modeling framework is now being extended to include more relevant intermediates, and the analyzed phase microstructures are being compared with the characterized phase morphologies by STXM measurements.

Task 5: Additives

The number of additives (e.g., transition metal halides and carbides) known to accelerate the kinetics of hydrogen desorption and uptake is large, but the mechanisms by which the rate increases are effected are largely unknown. Consequently, HyMARC investigations in this and prior years have focused on the most effective additives, in particular titanium halides (see Task 3), and on using additives as a tool to probe hydride chemistry. In the latter, we probed the mechanism of hydrogen uptake by MgB_2 . The rate-limiting step in the process to regenerate $\text{Mg}(\text{BH}_4)_2$ from this material was initially unclear but likely involved either B-B or H-H bond breaking. To probe this, we prepared samples of MgB_2 mixed with catalysts known to dissociate H_2 to form H atoms, including Fe, Pd, and WC. These additives did not significantly improve how fast MgB_2 reacted with H_2 indicating that H-H bond breaking is not the rate-limiting step. In a complementary experiment, the ability of these materials to break H-H bonds was directly measured with H-D isotopic exchange studies. These investigations showed that these additives, when combined with MgB_2 , break H-H bonds on a time scale that is fast compared to the slow hydrogenation of MgB_2 . Our results indicate that it is not H-H bond breaking

that is rate limiting, but disruption of the hexagonal B-B rings in MgB_2 or the formation of hydride (H^-) anions that limit the uptake of H_2 . Future investigations will focus on developing additive strategies addressing these possibilities.

Interactions with Seedling Projects and Collaborations

The SNL HyMARC team performed extensive measurements and testing in support of five seedling projects. More than 50 samples were exposed to hydrogen pressures ≥ 700 bar in SNL's ultrahigh-pressure reactor for two projects. In addition, XPS and porosimetry measurements were performed for two other projects, one of which resulted in a joint paper. Finally, SNL performed the go/no-go validation for two projects. Extensive collaborations with both U.S. and international organizations occurred, involving government and DOE national laboratories as well as universities.

CONCLUSIONS AND UPCOMING ACTIVITIES

Our research this year, in collaboration with LLNL and LBNL, enabled us to rank a number of material development strategies for sorbents and metal hydrides for their potential to meet DOE targets. The results of these studies were published [1, 2] and form the basis for the second phase of HyMARC, which commences in FY 2019. HyMARC will be reorganized in Phase 2 to incorporate three additional national laboratories (National Renewable Energy Laboratory, Pacific Northwest National Laboratory, and SLAC National Accelerator Laboratory), plus the National Institute of Standards and Technology Center for Neutron Research, with new research concentrated within specific “focus areas” that are the outgrowth of the research conducted in Phase 1. SNL will lead the overall effort on metal hydrides, including focus areas concentrating on atomistic simulations, experimental measurements of metal hydride thermodynamics, surfaces and solid-solid interfaces, additives, nanoscaling, and machine learning.

SPECIAL RECOGNITIONS AND AWARDS/PATENTS ISSUED

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Presentations

32 presentations (1 keynote and 20 invited) at national and international conferences and symposia were presented over the past 12 months.

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