IV.C.3 HyMARC (Core): LBNL Effort

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Phase I End Date: September 30, 2018

Overall Objectives

- Facilitate community discovery of light, high-capacity hydrogen storage materials and new materials strategies with fine control of nanoscale dimensions to meet weight and volume requirements via modalities such as encapsulation and confinement.
- Develop in situ and in operando soft X-ray characterization capabilities in combination with first-principles simulations to extract atomic and molecular details of functional materials and interfaces.
- Develop community tools and capabilities to enable materials discovery, including computational models and databases, new characterization tools and methods, and tailorable synthetic platforms.

Fiscal Year (FY) 2017 Objectives

- Develop graphene-encapsulated metal borohydride nanocrystal hydrides with control over material phase (alpha, beta, gamma) to produce environmentally-stable, high performance hydrogen storage materials. (This work is projected to aid the seedling project led by D.J. Liu from Argonne National Laboratory [ANL]).
- Control the size of metal hydride nanocrystals from 3–12 nm to provide model systems for hydriding/dehydriding phenomena for ongoing modeling efforts.
- Fabrication of an in situ X-ray spectroscopic gas flow cell to provide a new HyMARC capability able to be used to examine internal hydride interfaces dynamically during hydriding/dehydriding.
- Application of ex-situ X-ray absorption spectroscopy (XAS) to magnesium borohydride ($Mg(BH_4)_2$) to monitor changes in the local electronic structure indicative of kinetically limiting intermediates.
- Preparation of graphene nanoribbons featuring 1,10-phenanthroline ligands to test the hypothesis that functionalized carbons bearing binding sites for discrete metal complexes can catalyze hydrogen dissociation/association at the surface of the metal/metal hydride.
- Simulation and modeling of metal-graphene solid-solid interfaces to understand prototype metal hydride interfaces under oxidative and reductive environments.
- Identified the mechanistic role of functionalized graphene nanoribbons (GNRs) towards H_2 adsorption and dissociation in GNRs encapsulated Mg nanoparticles.
- Use first-principles modeling tools to deepen understanding of the surface structures of γ-$Mg(BH_4)_2$, which is thought to play a significant role in determining its practical performance.
- Deepen modeling efforts on hydride-graphene interfaces, in particular the interaction between graphene and cubic $NaBH_4$ (this work is in projected to aid the seedling project led by D.J. Liu from ANL).

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 Plan.

(O) Lack of Understanding of Hydrogen Physisorption and Chemisorption

(A) System Weight and Volume

(E) Charge/Discharge Rate

Technical Targets

This project does not have specific technical targets. However, some storage metrics are presented below after the discussion of HyMARC objectives.

Technical goal of HyMARC: This project will develop foundational understanding and new capabilities that will enable accelerated discovery of breakthrough materials in all classes of storage materials, in particular metal hydrides and sorbents. It is anticipated that the insights gained from this research, coupled with new synthetic, characterization, modeling, and database tools that will be made available to the hydrogen storage research community, will lead to materials that meet DOE targets such as system gravimetric and volumetric capacity, system fill time, and delivery temperature.

As mentioned, for context, Table 1 shows relevant storage metrics and how they stand in relation to some of the development of materials developed through this effort.

TABLE 1. Technical System Targets for Hydrogen Storage for Fuel Cell Vehicles

Storage Parameter	Units	DOE 2020	Ultimate
System Gravimetric Capacity	kWh/kg (kg H_2/kg System)	1.5 (0.045)	2.2 (0.065)
System Volumetric Capacity	kWh/L (kg H_2/L System)	1.0 (0.030)	1.7 (0.050)
Min/Max Delivery Temperature	°C	-40/85	-40/85
System Fill Time (5 kg)	minutes	3-5	3-5
Min/Max Delivery Pressure from Storage System	bar	5/12	5/12

This project is conducting studies on Mg nanocrystals encapsulated by reduced graphene oxide (rGO) layers. DOE hydrogen storage targets are quantified based on the system, while material-based numbers are presented.

- Gravimetric Capacity (based on the total material): 0.065 kg H_2/kg material
- Volumetric Capacity (based on the total material): 0.105 kg H_2/L material

FY 2017 Accomplishments

- Designed a graphene-encapsulation for different phases (γ, β, α) of magnesium borohydride ($Mg(BH_4)_2$) nanocrystals with a solution-based synthetic approach (Figure 1). This is based upon prior Mg/rGO work in the Urban group.
- Prepared $Mg(BH_4)_2$ nanocrystals encapsulated by rGO layers which releases 10.2 wt% H_2 in terms of the total material weight. Investigated the effect of different rGO loading on the hydrogen desorption properties (Figure 2).
- Established the role of thin interfacial oxide layer in contributing stronger binding between reduced graphene oxide and the Mg nanoparticle, thus improving the mechanical and chemical stability of the functioning nanocomposite without hindering the overall hydrogenation-dehydrogenation process.
- Developed instrumentation: The new soft X-ray in situ gas flow cell is now under commissioning at the Advanced Light Source (ALS). It gives better temperature control on the sample surface (room temperature to 300°C). In addition, this new gas cell has better gas sealing for evacuating the sample environment. Figure 3 shows the design drawing of the new version of the in situ X-ray spectroscopic gas flow cell. The gas cell has been fabricated and is currently under testing in order to examine its working temperature range, vacuum/gas sealing and safety.
- Studied pristine and hydrogenated $LiBH_4$ by ex situ XAS at B K-edge with possible intermediate products such as $Li_2B_{12}H_{12}$ (Figure 4). Furthermore, a series of reference samples, including Li_3N, $LiNH_2$ and $LiNH_3$, were studied at N K-edge XAS for future XAS spectra database use.
- Discovered that the improvement of H_2 uptake processes (both H_2 adsorption and dissociation) in nitrogen-functionalized GNR (4N-GNR)/Mg nanocomposite is due to interfacial interactions that create a number of undercoordinated, slightly oxidized Mg (Figure 5).
- Studied various surface terminations of γ-$Mg(BH_4)_2$ (001) surface. The thermodynamically most stable surface was found to be the BH_4^- terminated surface with low BH_4^- coverage. When the BH_4^- coverage increases, it spontaneously transforms into a $B_2H_7^-$ terminated surface by releasing H_2 gas.

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INTRODUCTION

Storage of hydrogen onboard vehicles is one of the critical enabling technologies for creating hydrogen-fueled transportation systems that can provide U.S. energy independence and abate air pollution. 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. Nevertheless, solid-state materials, including novel sorbents and high-density hydrides, remain of interest because of their unique potential to meet all Fuel Cell Technologies Office targets and deliver hydrogen at lower pressures and higher onboard densities. A successful solution would significantly reduce costs and ensure the economic viability of a U.S. hydrogen infrastructure.

LBNL's effort within HyMARC is to provide leadership to the LBNL effort of HyMARC as well as Task 4 (solid-solid interfaces). The LBNL effort also seeks to develop (via multidisciplinary and multi-lab collaborations) novel materials platforms and cutting-edge, in situ characterization to reveal key functional aspects of various materials components in enhancing the efficiency and stability of hydrogen storage. By focusing on encapsulation, protection, or confinement of active materials within lightweight, selectively permeable, functional media, we have realized advances in the performance of model systems, specifically

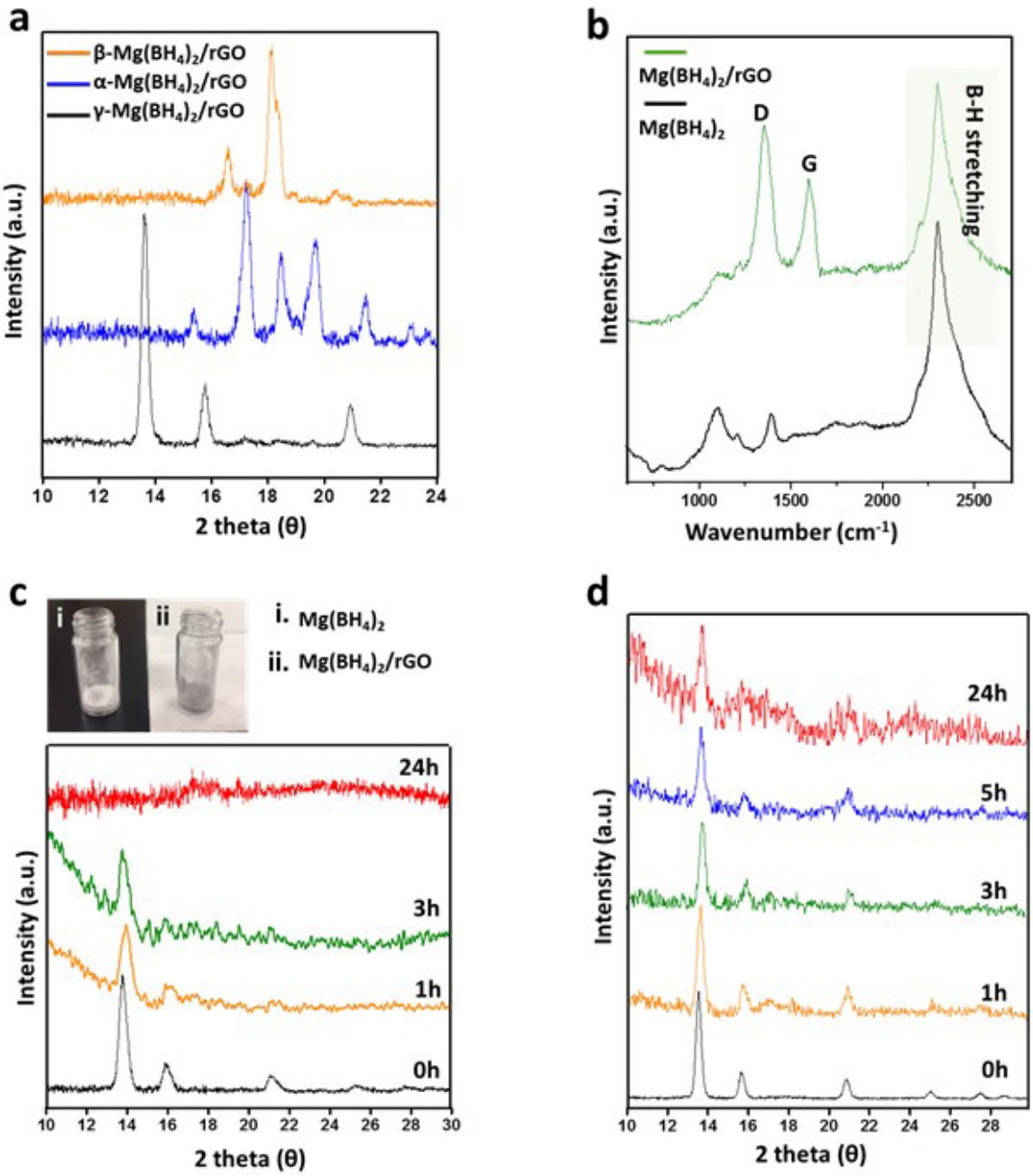

FIGURE 1. (a) X-ray diffraction patterns of β-, α-, γ-$Mg(BH_4)_2$/rGO heterostructures. (b) Raman spectra of $Mg(BH_4)_2$ and $Mg(BH_4)_2$/rGO heterostructures. The Raman spectrum of $Mg(BH_4)_2$/rGO displays B-H stretching of $Mg(BH_4)_2$ which is well matched with bulk $Mg(BH_4)_2$ and the D and G band of rGO at between at 1,300 cm^{-1} and 1,700 cm^{-1}. Air stability of $Mg(BH_4)_2$ without (c) and with (d) rGO. $Mg(BH_4)_2$/rGO composites show better air stability compared to $Mg(BH_4)_2$ without rGO. Photograph of white powder of $Mg(BH_4)_2$ (c inset, i) and grey powder of $Mg(BH_4)_2$/rGO (c inset, ii).

magnesium wrapped in rGO, and are seeing similar gains in complex borohydrides (Tasks 1 and 2). The same systems are being analyzed using unique in situ X-ray spectroscopic probes, such as XAS, that reveal depth-dependent and interfacial chemical composition at various stages of loading with hydrogen and throughout the history of cycled materials (Tasks 3 and 4). Furthermore, such systems can be understood in atomic and electronic detail using first-principles calculations, consistent with characterization, that reveal the important role of materials interfaces in controlling the kinetics and stability of thermodynamically well-defined storage systems (Task 2), or perhaps alter

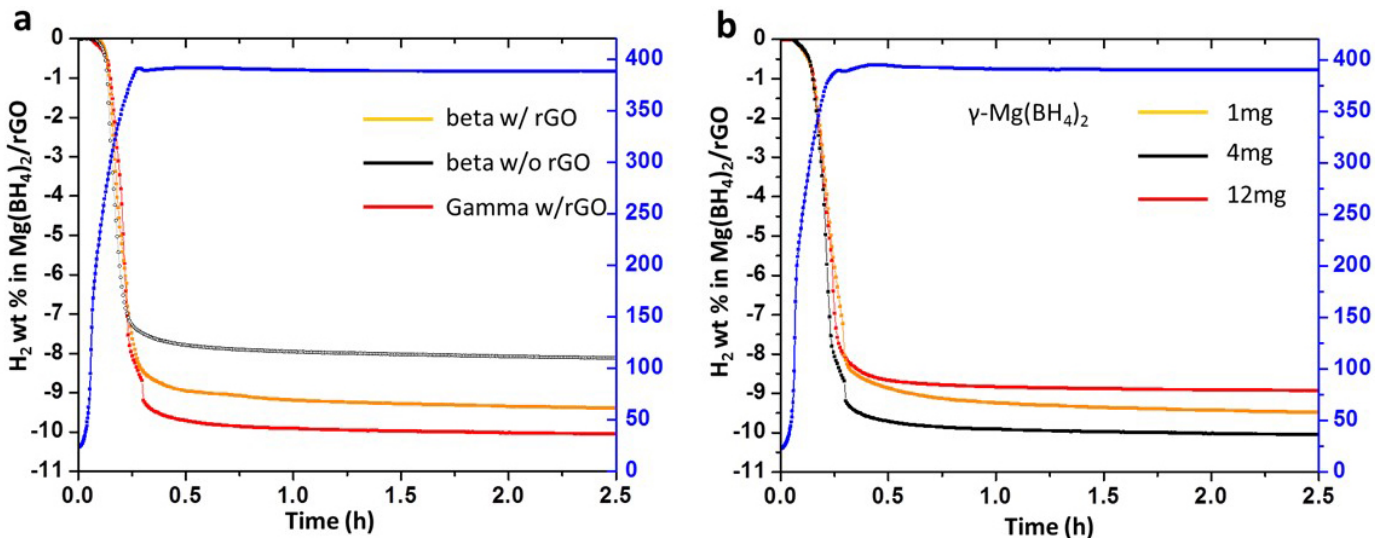

FIGURE 2. Hydrogen desorption (at 390°C and 0 bar) for the as-synthesized $Mg(BH_4)_2$/rGO. (a) γ-$Mg(BH_4)_2$/rGO releases a large amount of hydrogen (10.2 wt%). In addition $Mg(BH_4)_2$ without rGO less released hydrogen (8.1 wt%) compared to $Mg(BH_4)_2$ with rGO. (b) γ-$Mg(BH_4)_2$ with rGO loading of 4 mg shows the best hydrogen desorption performance.

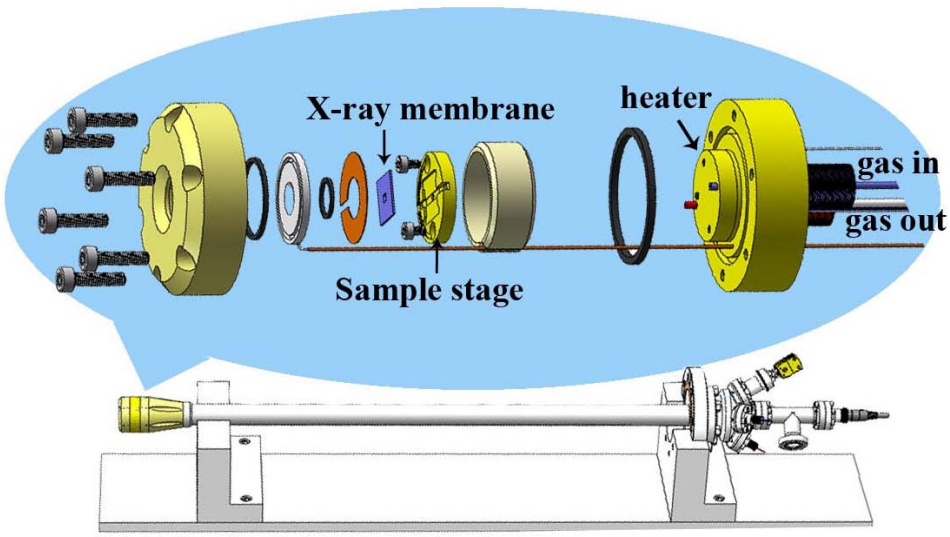

FIGURE 3. The in situ X-ray spectroscopic gas flow cell design drawing. The design specification for the cell are; provide higher accuracy and stability in temperature on sample surface to 300°C, improve better gas and vacuum sealing ideal for hydrogen dehydronation process.

the thermodynamics by defining interphases with distinct energetics, such as the interfacial suboxide in rGO-encapsulated magnesium (Task 1). Incorporation of additives (transition metals in magnesium) or chemical functional groups within confining media (N and O functionalization of GNRs) to enhance activity is being explored synthetically and theoretically (Task 5). Finally, we are engaged in large scale investigations of sorbent databases using empirical modeling to derive descriptors for hydrogen storage that can guide materials development (Task 6). The expertise gained in each of these efforts is available to seedling projects and already being utilized by efforts related to graphene encapsulation of complex hydrides (Liu, ANL) and etherate additives in the $MgB_2/Mg(BH_4)_2$ system (Severa, University of Hawaii).

APPROACH

HyMARC seeks to overcome the lack of foundational understanding that is key to materials systems advances in increasing efficiency and stability of hydrogen storage through our integrated studies of model systems and

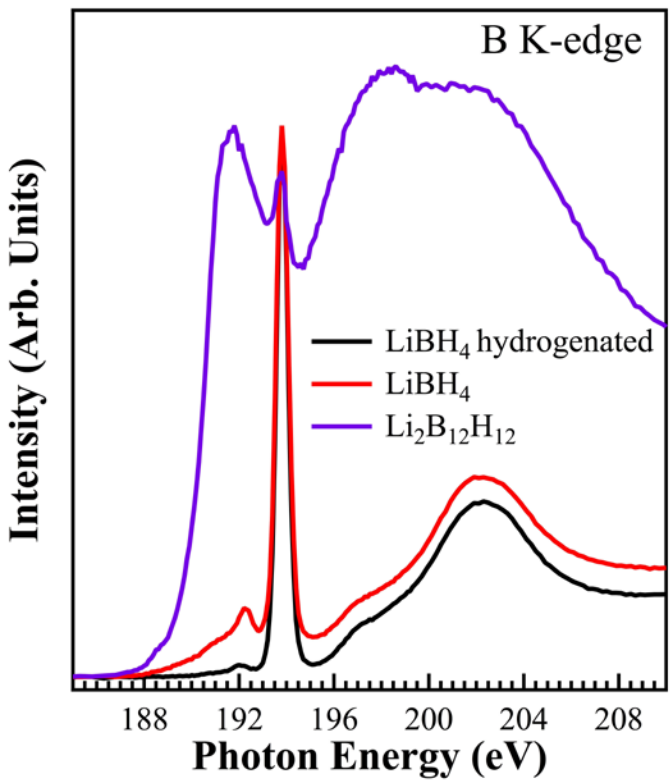

FIGURE 4. Boron K-edge XAS spectra of $LiBH_4$ (pristine and hydrogenated $LiBH_4$ under 70 bar at 400°C) with reference sample $Li_2B_{12}H_{12}$ are presented. A very small portion of $Li_2B_{12}H_{12}$ may present in $LiBH_4$, which recently been observed by NMR experiment from Stavila. The presence of $(BH_4)^{2-}$ ion is considered responsible to the degradation of reversibility. Therefore, possible intermediate $Li_2B_{12}H_{12}$ could form in hydrogenated process.

promising materials classes using synthesis, characterization, and theory and modeling. The LBNL component of the HyMARC team leverages expertise in chemical and materials synthesis, X-ray spectroscopic characterization, first-principles theory and modeling and force-field based exploration of materials databases.

RESULTS

Substantial results on all tasks were made, and nearly all quarterly goals were met on time. LBNL principal investigators led or co-led task groups and helped coordinate and participate in meetings. In addition to managerial output, the key technical results were as follows:

Complex hydride synthesis: This is a key result, translating the approaches developed on model Mg hydride materials to higher capacity borohydrides. A rGO-encapsulation strategy was developed to provide phase control for different phases (γ, β, α) of $Mg(BH_4)_2$ nanocrystals with a solution-based synthetic approach (Figure 1). Because $Mg(BH_4)_2$ is one of the highest-capacity hydrogen storage materials (14.9 wt%) known, this is a key step toward robust high-capacity systems. This nano-hybrid system is important for understanding how solid-solid interfaces impact absorption/desorption kinetics and provide a reaction pathway to improved kinetics.

The stability and performance of these materials were studied as well. The air stability of γ-$Mg(BH_4)_2$ with and without rGO was studied to prove that rGO is able to show the high gas selectivity that is sufficient to discriminate between H_2 and other molecules (H_2O, O_2) (Figure 1c and 1d). The performance of prepared $Mg(BH_4)_2$ nanocrystals encapsulated by rGO layers was performed in collaboration with Stavila (SNL), demonstrating the release of 10.2 wt% H_2 in terms of the total material weight (Figure 2a). This system is now approaching the theoretical capacity value (14.9%) of $Mg(BH_4)_2$. Further, the effect of different rGO loadings on the hydrogen desorption properties was investigated to learn how the amount of rGO impacts desorption kinetics and thermodynamics (Figure 2b).

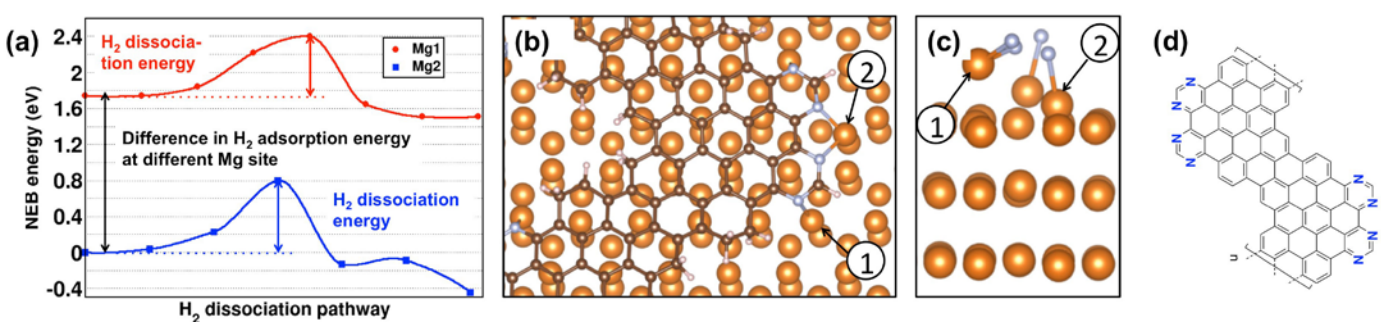

FIGURE 5. (a) H_2 dissociation energy at different Mg sites in 4N-GNR/Mg nanocomposite. (b) The structure of 4N-GNR/Mg (top view). The Mg atoms, marked as 1 and 2, are moving outward to directly bond with N from the 4N-GNR and the H_2 dissociation energy on these Mg atoms is calculated using the climbed imaging nudged elastic band (NEB) methods in (a). (c) Side view of the 4N-GNR/Mg structure. (d) The structure of 4N-GNR. In these structure representations, Mg, C, N and H are shown as orange, brown, light blue, and pink spheres, respectively.

Results in sorbents–modeling and synthesis: Efficient and accurate determination of the volumetric and gravimetric capacity of nanoporous adsorbents at hydrogen fueling (100 bar) and delivery (5 bar) pressures is key to materials selection and development for onboard hydrogen storage applications. We have analyzed the variance in simulated hydrogen isotherms in nearly 500 metal-organic frameworks (MOFs) due to model inputs such as classical H_2 potentials, equations of state for H_2, and density functional theory-based optimization of experimentally-derived MOF structures. Our high-throughput analysis revealed a strong correlation between total H_2 adsorption at 100 bar and MOF void volume that outperforms a well-known correlation between H_2 adsorption and surface area.

Furthermore, it was determined that the coverage of hydrogen is the same for the neutral MCF-17 mesoporous silica as for the acidified MCF-17 (Al-MCF-17) with two different concentrations of acidic sites (Al-MCF-17 with Si:Al ratio of 11:1 and 57:1) (Figure 6). Nevertheless, the concentration of acidic sites (Brønsted and Lewis) was found to affect the heat of adsorption determined from low temperature adsorption studies (-50°C to -90°C) as presented in Table 2. The primary goal of this work was to understand how charges or acidic protons affect the heat of hydrogen adsorption.

Application of X-ray spectroscopic capabilities: Advancing the performance of these capabilities is essential to understanding the role that internal solid-solid interfaces and transient intermediates play in hydrogen storage. Soft X-ray spectroscopy and imaging characterization measurements were carried out with Jinghua Guo at the ALS working closely with the HyMARC teams of Tasks 1, 3, 4, 5. We have characterized air-stable γ-$Mg(BH_4)_2$ nanocomposites and several solid-state metal hydrides ($Mg(BH_4)_2$, Li_3N, Li_2NH, and $LiNH_2$, $LiBH_4$, LiH, $Li_2B_{12}H_{12}$, $LiAlH_4$, LiOH, and $LiBH_4$). These efforts assist the foundational understanding of the relevant physical and chemical interactions occurring on the spatial scale of atoms and molecules with solid-state metal hydrides.

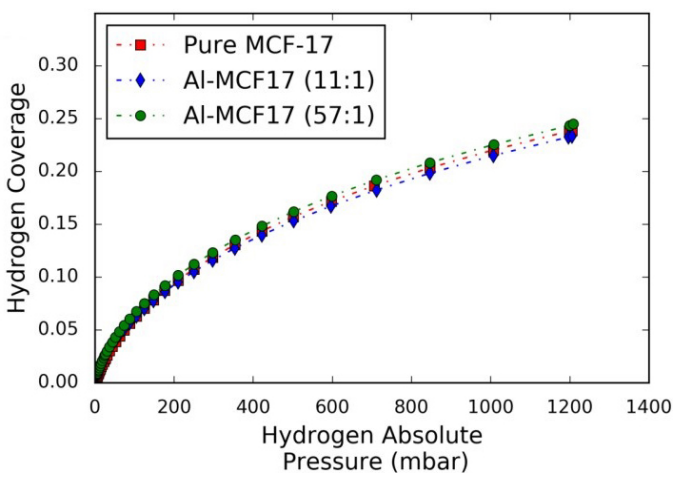

FIGURE 6. Normalized hydrogen adsorption in terms of coverage on neutral (MCF-17) and acidified (Al-MCF-17) mesoporous silica with different concentration of aluminum (or acidic) sites. The measurements were carried out at 77 K.

TABLE 2. Heat of Adsorption for Neutral and Acidified Mesoporous Silica and for Carbon as a Standard Sample

Samples	Surface area (m^2/g)	Heat of Adsorption (kJ/mol of H_2)
Carbon	930.0	8.4
MCF-17		4.5
Al-MCF-17 (57:1)	322.8	2.9
Al-MCF-17 (11:1)	498.5	4.9

Specific highlights include the ex situ XAS characterization of α-, β-, and γ-$Mg(BH_4)_2$, both with and without rGO encapsulation, including both the pristine and dehydrogenated γ-phase. Mg K-edge spectra of γ-$Mg(BH_4)_2$ with and without rGO capsulation is shown in Figure 7. We studied pristine and hydrogenated $LiBH_4$ by ex situ XAS at B K-edge with possible intermediate products such as $Li_2B_{12}H_{12}$ (Figure 4). The access to the soft X-ray region of B K-edge is more critical now owing to results from the previous year. Furthermore, a series of reference samples were studied at N K-edge XAS, including Li_3N, $LiNH_2$ and $LiNH_3$, for future XAS spectra database use.

Development of new X-ray in-situ instrumentation: The new soft X-ray in situ gas flow cell is now under commissioning at the ALS. It provides better temperature control on the sample surface (room temperature to 300°C). In addition, this new gas cell has better gas sealing for evacuating the sample environment. Figure 3 shows the design drawing of the new version of the in situ X-ray spectroscopic gas flow cell. The gas cell has been fabricated and is currently under testing in order to examine its working temperature range, vacuum/gas sealing and safety.

Accomplishments in additives: In an effort to lower the activation temperature for H_2 adsorption and desorption in metal hydrides we developed a stabilizing GNR matrix that is functionalized with molecularly defined hydrogen dissociation catalysts (Task 5). The close proximity of these catalysts to the metal surface (the site of hydrogen uptake) increases the local concentration of hydrogen atoms during the uptake process. The principle of microscopic reversibility allows the same catalyst to lower the barrier for hydrogen atom recombination during the H_2 release. These study of these catalytic GNRs will allow us to decouple the kinetic contribution from diffusion/effusion in the solid from the H_2 dissociation reaction at the surface of different metals. We successfully introduced transition metal complexes along the edges of 1,10-phenanthroline functionalized GNRs (Figure 8). In an initial effort to optimize the reaction conditions and monitor the progress, the coordination

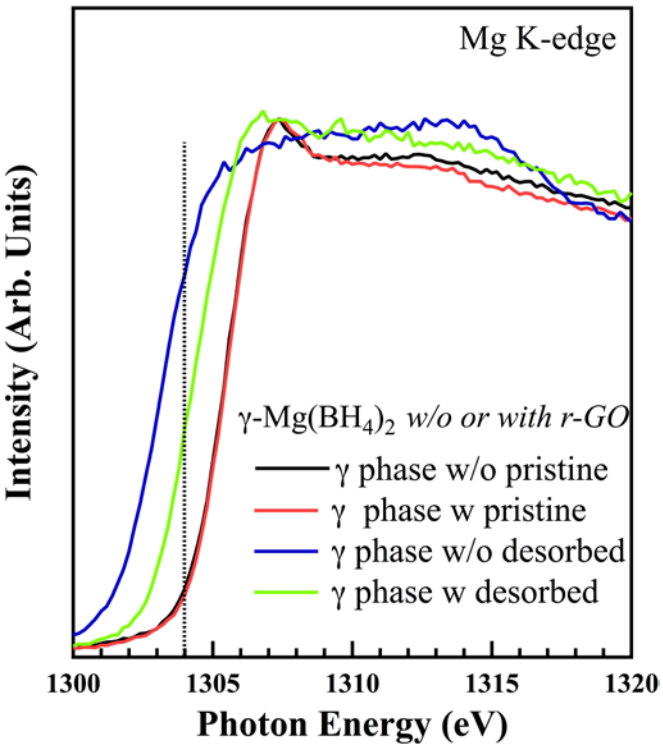

FIGURE 7. Mg K-edge XAS spectra of pristine and hydrogen desorbed $Mg(BH_4)_2$ without or with rGO capsulation. The dotted line indicates the lower onset in energy upon hydrogen desorption, i.e., black and blue curves. The earlier onset is also observed in MgB_2, which is not shown in this figure. Hence, the different onset in spectra between without and with rGO $Mg(BH_4)_2$ are indicating that the rGO layer plays an important role in kinetics. In addition, it is also clear evidence that $MgB_{12}H_{12}$ is not present after hydrogen desorption since the early onset is absent in the spectrum. The XAS results indicate that $MgB_{12}H_{12}$ is not present which is harmful to reversibility during hydrogen desorption/absorption process.

of $Re(CO)_5Cl$ (a known catalyst capable of activating dihydrogen) to the 1,10-phenanthroline decorated GNRs was studied. The resulting complex, a $Re(CO)_3Cl$(phenanthroline), features three carbonyl groups that were used as characteristic markers in infrared spectroscopy. Thermogravimetric analysis and elemental analysis indicate that under the optimized reaction conditions, the yield of metallated 1,10-phenanthroline groups in GNRs exceeds 99%. Current work is dedicated to expanding the variety of transition metal based hydrogenation catalysts (Pt, Pd, Ni, Rh, Ir) that can be coordinated to the functionalized GNRs. The process of developing a standard reaction protocol to benchmark the activity of the respective GNR heterostructure hydrogenation complexes is underway in collaboration with Lennie Klebanoff of Sandia National Laboratories.

Results in theory and simulation of solid-solid interfaces: Within the context of graphene or rGO encapsulation as a means to protect nanoparticles of active materials from oxidizing environmental agents (e.g., oxygen, water) and provide a selectively permeable membrane for H_2, we noted the presence of some oxidation in model Mg nanoparticle systems based on XAS measured at the ALS. Using first-principles calculations of both atomistic models and associated simulated spectra (a capability available within HyMARC) we established the role of an atomically thin interfacial oxide layer in contributing stronger binding between rGO and the Mg nanoparticle, thus improving the mechanical and chemical stability of the functioning nanocomposite without hindering the overall hydrogenation-dehydrogenation process.

First-principles calculations revealed improvements in H_2 uptake (both H_2 adsorption and dissociation) in 4N-GNRs encapsulating Mg, synthesized by Fischer. There is a strong interfacial interaction that creates a number of undercoordinated, slightly oxidized Mg atoms at the metal nanoparticle surface, which are active sites of H_2 uptake (Figure 5). Moving towards higher capacity complex hydrides, we used first-principle calculations to study various surface terminations of the γ-$Mg(BH_4)_2$ (001) surface, finding the thermodynamically most stable surface to be the BH_4^- termination with low BH_4^- coverage. When the BH_4^- coverage increases, it spontaneously transforms into the $B_2H_7^-$ terminated surface by releasing H_2 gas indicating intrinsic activity of this surface. In relation to the Liu (ANL) HyMARC seedling project, we determined using first-principles calculations that weak graphene/$NaBH_4$ interactions are generally found at different $NaBH_4$ surfaces, except for the Na-terminated $NaBH_4$ (111) surface.

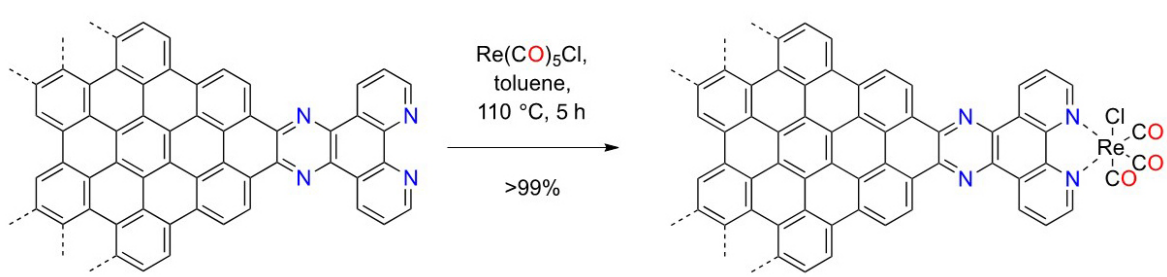

FIGURE 8. Synthetic scheme detailing the integration of molecularly defined transition metal complexes along the edges of functional GNRs.

CONCLUSIONS AND UPCOMING ACTIVITIES

Our team has interacted closely with the other HyMARC partners and new seedling projects to build foundational understanding of thermodynamics and kinetics in solid-state hydrogen storage materials. This year we met a key goal, transitioning our synthetic activities from model Mg hydrides to more complex and higher capacity Mg borohydrides. Other synthetic work aims to use functionalized carbon materials to protect hydrides from degradation while also providing catalytic enhancement of kinetics via targeted placement of transition metal species. On the characterization side, our investigations into hydride interfaces using soft X-ray probes continue, with development of in situ cells being a substantial advance. On the theory side, we discovered that sub-oxide interfacial chemistry plays a surprisingly beneficial role in metal hydride kinetics and reversibility. Further, the modeling work on the MOF database has expanded and will soon be ready to make testable predictions of the thermodynamics and capacity of new porous materials. In the coming months, we aim to:

- Optimize the thermodynamics and kinetics of the dehydrogenation and hydrogenation processes of encapsulated $Mg(BH_4)_2$/rGO hybrid nanomaterials (collaboration with the seedling project at ANL).
- Extend our study of the chemical stability of γ-$Mg(BH_4)_2$ towards oxidation and water contamination and more fully explore the interfacial interaction between γ-$Mg(BH_4)_2$ and graphene, based on the surprising beneficial role of limited oxidation in model Mg NP/rGO composites and initial studies of pristine stable surface terminations.
- Use first-principles molecular dynamics to examine the thermodynamics and kinetics of the dehydrogenation process in etherated $Mg(BH_4)_2$ (collaboration with the seedling project at the University of Hawaii).
- Continue to develop multivariate linear models to correlate MOF pore descriptors (pore volumes, cavity diameters, cavity curvature) to H_2 adsorption at other temperature and pressure conditions (5 bar, near-ambient temperatures). These models will enable rapid characterization of H_2 storage performance at both storage and delivery conditions. This effort will place particular emphasis on MOFs with coordinately unsaturated ("open") metal sites, supporting the University of California, Berkeley seedling project.
- Utilize the new Advanced Materials Beamline for Energy Research (AMBER 6.0.1) at the ALS, in use starting April 2018, which will offer a new capability for the entire HyMARC effort.
- Continue building on the demonstration that molecularly defined hydrogen dissociation catalysts can be seamlessly integrated into a functional GNR/metal nanoparticle composite material. This technology will enable us to decouple the H_2 dissociation kinetics from the diffusion dynamics that dominate uptake and release kinetics in metal hydrides. Our next steps will establish the benchmark kinetics for catalyst modified GNRs (Task 5 in collaboration with Lennie Klebanoff, Sandia National Laboratories) and study the change in the uptake/release kinetics for metal hydride composites (initial experiments will rely on the MgH_2 and AlH_3 system established through our work in Task 4).

SPECIAL RECOGNITIONS & AWARDS/ PATENTS ISSUED

1. (Urban) SBIR awarded for H_2 storage work with Agiltron, Inc. (scale up of metal hydrides).

2. (Urban) New PCT filed on H_2 work partially supported by HyMARC: 2015-089-02 H_2 storage laminates.

3. (Urban) New provisional patent filed on H_2 work partially supported by HyMARC: 2013-065-01 doped nanostructures for H_2 storage.

FY 2017 PUBLICATIONS/PRESENTATIONS

Publications

1. "Atomically-thin interfacial suboxide key to hydrogen storage performance enhancements of magnesium nanoparticles encapsulated in reduced graphene oxide," Liwen F. Wan, Yi-Sheng Liu, Eun Seon Cho, Jason D. Forster, Sohee Jeong, Hsiao-Tsu Wang, Jeffrey J. Urban, Jinghua Guo, and David Prendergast, *accepted*, *Nano Letters*.

2. "Tailoring polymer configuration for nanocrystal growth: the role of chain length and solvent," Eun Seon Cho, Fen Qiu, and Jeffrey J. Urban, *Small,* **13(3)**, (2017). DOI: 10.1002/smll.201602572. This article is featured on the frontispiece (inside cover) of *Small,* 13(3), (2017).

3. "Graphene ribbon nanobelted Mg crystals for high capacity hydrogen storage," Eun Seon Chô, Tomas Marangonî, Yi-Sheng Liu, Cameron Rogers, Edmond W. Zaia, Ryan R. Cloke, Patrick T. Shea, Yi-De Chuang, Jinghua Guo, Brandon C. Wood, Felix R. Fischer*, and Jeffrey J. Urban*, *submitted* (2017).

4. "Hierarchically controlled inside-out doping of Mg Nanocomposites for moderate temperature hydrogen storage," Eun Seon Chô, Anne M. Ruminski, Yi-Sheng Liu, Patrick T. Shea, ShinYoung Kang, Edmond W. Zaia, Yi-De Chuang, Xiaowang Zhou, Tae Wook Heo, Jinghua Guo, Brandon C. Wood, and Jeffrey J. Urban, *under revision, Advanced Functional Materials* (2017).

Presentations

Jeffrey J. Urban:

1. May 2017 – ECS National Meeting, New Orleans, LA (Invited keynote).

2. January 2017 – Invited talk at ALS-U workshop, Berkeley, CA.

3. October 2016 – ECS National Meeting, Honolulu, HI (Invited).

4. September 2016 – Department of Civil Engineering, Berkeley, CA.

Felix R. Fischer:

1. Max Planck Gesellschaft – Conference on Molecular Nanostructures, Ascona, Switzerland, February 6–10, 2017.

2. Polymers Gordon Research Conference, Mt. Holyoke College, U.S.A., June 11–16, 2017.

3. Physical Organic Chemistry Gordon Research Conference, Holderness School, U.S.A., June 25–30, 2017.

4. International Conference on Novel Aromatics, Stoney Brook, U.S.A., July 23–28, 2017.

Jinghua Guo:

1. "In-Situ/Operando Soft X-Ray Spectroscopy of Catalytic and Electrochemical Reactions," The 252nd ACS National Meeting, symposium: Advanced Nanoscale Chemical Imaging of Catalyst Materials, Philadelphia, PA (August 21–25, 2016).

2. "In-Situ/Operando Soft X-Ray Spectroscopy of Catalytic and Electrochemical Reactions," SPIE 2016 Optics + Photonics for Sustainable Energy, symposium: Solar Hydrogen and Nanotechnology XI, San Diego, CA (August 28–September 1, 2016).

3. "In-Situ/Operando Resonant Inelastic Soft X-ray Scattering Characterization of Chemical and Catalytic Reactions," Department of Chemistry, Materials Science & Engineering, University of California, Berkeley, CA (September 23, 2016).

4. "Synchrotron Radiation Based Soft X-ray Characterization of Energy Materials," invited lecture, Tokyo University of Science, Japan (December 22, 2016).