HyMARC: A Consortium for Advancing Solid-State Hydrogen Storage Materials

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## Overview (LBNL)

<table>
<thead>
<tr>
<th>Timeline</th>
<th>Barriers addressed</th>
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</table>
| **Project start date:** 09/21/2015  
**Phase I end date:** 09/30/2018 | • Lack of understanding of hydrogen physisorption and chemisorption (Barrier O)  
• System weight and volume (Barrier A)  
• Charge/discharge rate (Barrier E) |

<table>
<thead>
<tr>
<th>Budget</th>
<th>Team</th>
</tr>
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</table>
| FY17 DOE Funding: $770K  
FY18 DOE Funding: $775K  
Total Funds Received: $2.585M (all years) | **Funded Partners:**  
Sandia National Laboratories (lead)  
Lawrence Livermore National Laboratory |
Relevance and Objectives

HyMARC will provide **community tools** and **foundational understanding** of phenomena governing thermodynamics and kinetics to enable development of solid-phase hydrogen storage materials.

**Theory, simulation, & data**
- Quantum Monte Carlo for sorbents
- DFT and *ab initio* molecular dynamics for bulk/surface/interface chemistry
- Classical MD & kinetic Monte Carlo for non-equilibrium transport
- Phase-field modeling for solid-state phase transformation kinetics
- Computational spectroscopy
- Community software & databases

**Controlled synthesis**
- Metal organic frameworks (MOFs)
- Hierarchical integrated bulk and nanoscale metal hydrides
- High-pressure synthesis
- Functionalized carbon encapsulants and porous nanoconfining media
- Sorbent suite for model testing and validation

**In situ characterization**
- Ambient-pressure XPS
- Soft X-ray absorption and emission spectroscopy
- Electron microscopy and X-ray spectromicroscopy
- Low-energy ion scattering for surface hydrogen detection
Project Objectives, overall:

- Focus on **light materials** and synthesis strategies with fine **control of nanoscale dimensions** to meet weight and volume requirements via encapsulation, confinement (A)
- Design **interfaces with chemical specificity** for thermodynamic and kinetic control (E) of hydrogen storage/sorption and selective transport
- Explore **novel storage concepts** and/or obtain **fundamental understanding** of “established” processes via known/idealized systems/materials (O)
- Develop in situ/operando **soft X-ray characterization** capabilities in combination with **first-principles simulations** to extract atomic/molecular details of functional materials and interfaces (O)
- Refine chemical synthesis strategies based on atomic/molecular scale insight from characterization/theory

*Establish expertise and capabilities for the H₂ storage community*
Relevance

**FY18 Project Objectives:**

- Develop more complete model for metal hydride-graphene interface based upon in-situ X-ray spectroscopy and theoretical modeling
- Develop synthesis of pure Mg(BH$_4$)$_2$ NPs wrapped by rGO
- Advance tools to enable in-situ X-ray spectroscopic experiments on buried interfaces in metal hydrides in different working temperature region
- Develop synthesis to enable targeted extrinsic doping using graphene nanoribbon based systems
- Perform accurate simulations of high-pressure H$_2$ sorption in MOFs based upon information from CoRE database
Technical Approach: Contributions of LBNL to HyMARC, Integration Across All Tasks, Access to All Labs

<table>
<thead>
<tr>
<th>Tasks</th>
<th>LBNL Team:</th>
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<tbody>
<tr>
<td>2,3,4,5</td>
<td>Jinghua Guo (<a href="mailto:jguo@lbl.gov">jguo@lbl.gov</a>): X-ray synchrotron spectroscopy</td>
</tr>
<tr>
<td>2,3,4,5</td>
<td>David Prendergast (<a href="mailto:dgprendergast@lbl.gov">dgprendergast@lbl.gov</a>): Computational spectroscopy</td>
</tr>
<tr>
<td>1,4</td>
<td>Jeff Urban (<a href="mailto:jjurban@lbl.gov">jjurban@lbl.gov</a>): Phase transitions and nanoscale effects in hydrides</td>
</tr>
<tr>
<td>1,5</td>
<td>Gabor Somorjai (<a href="mailto:gasomorjai@lbl.gov">gasomorjai@lbl.gov</a>): Functional sorbents</td>
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<tr>
<td>1</td>
<td>Felix Fischer (<a href="mailto:ffischer@lbl.gov">ffischer@lbl.gov</a>): Functionalized graphene nanoribbons</td>
</tr>
<tr>
<td>6</td>
<td>Maciek Haranczyk (<a href="mailto:mharanczyk@lbl.gov">mharanczyk@lbl.gov</a>): Materials genome for porous materials</td>
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Entire HyMARC Team accessing LBNL BES User Facilities

**The Molecular Foundry (TMF):**
- synthesis, characterization, and simulation of nanoscale materials/interfaces
- National Center for Electron Microscopy
- access to supercomputing (NERSC) through existing Foundry allocations

**Advanced Light Source (ALS):**
- Soft X-ray absorption/emission spectroscopies (XAS/XES) – in situ
- Ambient Pressure XPS
- Scanning Transmission X-ray Microscopy (STXM) and Ptychography

**Active user projects at TMF and ALS and Approved Program Proposal @ ALS**
- partnership to foster a new soft X-ray H$_2$ storage user community

- Enabling approach: **user projects acquired for Molecular Foundry and ALS**
- Innovative synthetic routes to metal hydrides and hybrid nanoscale systems to reveal key phenomena governing H₂ release/absorption and motivate new H₂ storage materials
- Developing new acid/base concepts to modify the enthalpy of H₂ binding in sorbents
- Creating algorithms to enable computation of H₂ isotherms in framework materials
- **In-situ** spectroscopic and structural characterization techniques that establish the role of interfaces in controlling H₂-storage reaction mechanisms and pathways;
- Computational modeling of structure, chemistry and dynamics of interfaces and additives for nanoscale H₂ storage systems and interpretation of X-ray spectroscopy
Accomplishment: Synthetic control over Mg(BH₄)₂ nanoparticle phase

- Tasks 1, 4 (Urban)

- First achievement of the pure phase control in encapsulated Mg(BH₄)₂/rGO materials
- Development of the facile synthetic method for 3 different phases (alpha, beta, gamma) of Mg(BH₄)₂
Accomplishment: Reversibility in $\gamma$-Mg(BH$_4$)$_2$/rGO – Tasks 2,3,4 (Urban)

i. Mg(BH$_4$)$_2$/rGO( MBHg) ii. Dehydrogenated MBHg iii. Rehydrogenated MBHg

Accomplishment: Reversibility in $\gamma$-Mg(BH$_4$)$_2$/rGO – Tasks 2,3,4 (Urban)

Our Mg(BH$_4$)$_2$/rGO hybrids also show reversibility for alpha/beta phases - not demonstrated in literature.
Accomplishment: in-situ XAS cell developments for Hydrogen storage - Tasks 1, 3, 4, 5 (Guo)

In-situ flow gas cell (1 bar, max. 400°C)

Quasi solid-gas cell (UHV, max. 500°C)

- Multimodal in-situ/quasi gas cells have developed for studying gas/solid interaction in different working temperature region and adoptable to varying beamlines in the ALS.

- Material based H₂ absorption/desorption and CO₂ capture can be studied using in-situ/quasi XAS technique.

- Proposed experiments in progress from Urban’s Group. (Mg(BH₄)₂)
Accomplishment: Ex situ characterization on metal borohydrides—Task 3,4,5 (Guo, Stavila, Klebanoff)

XAS characterizations have been applied on Mg, B, C, N, O K-edge and Ti, Fe L-edges for nano, TiF₃/TiCl₃, Fe, Tungsten Carbide (WC) catalyzed MgB₂. (collaborative with L. E. Klebanoff and V. Stavila from Sandia)

Fe or TiF₃ doped MgB₂

TEY – surface sensitive
TFY – bulk sensitive

consistent evidence for boron oxidation within these samples

less clear for Fe
Accomplishment: Ex situ characterization on metal borohydrides—Task 3,4,5 (Guo, Stavila, Klebanoff)

XAS characterizations have been applied on Mg B, C, N, O K-edge and Ti, Fe L-edges for nano, TiF$_3$/TiCl$_3$, Fe, Tungsten Carbide (WC) catalyzed MgB$_2$. (collaborative with L. E. Klebanoff and V. Stavila from Sandia)

Nano MgB$_2$

Tungsten Carbide additive

TEY – surface sensitive
TFY – bulk sensitive

Oxidation in Nano MgB$_2$

Carbides appear to remain intact – no clear evidence for graphite phase sep’n
Accomplishment: Ex situ characterization on metal borohydrides—Task 3, 4, 5 (Guo, Stavila, Klebanoff)

XAS characterizations have been applied on Mg B, C, N, O K-edge and Ti, Fe L-edges for nano, TiF$_3$/TiCl$_3$, Fe, Tungsten Carbide (WC) catalyzed MgB$_2$. (collaborative with L. E. Klebanoff and V. Stavila from Sandia)


L. E. Klebanoff et al, in preparation

TEY – surface sensitive
TFY – bulk sensitive

Analysis ongoing for ex situ N K-edge in prep for STXM

B oxidation ever present
Accomplishment: In-situ XAS investigation in Mg hydrides - *Tasks 4 (Guo, Urban)*

- Ni-doped rGO-Mg shows enhanced kinetic, the in-situ XAS characterization showing Mg hydride detected at 1 bar H₂ environment.

Ex-situ: Mg(BH₄)₂

S. Jeong et al., in prep.

First XPS study of Mg(BH₄)₂ to our knowledge

S. Jeong et al., in prep.

**In-situ Mg XAS experimental sequence from top to bottom**

In-situ spectra zoom-in in pre-edge region. Disappearing XAS feature indicates hydride formation. (arrow)
Accomplishment: In situ characterization on Mg(BH$_4$)$_2$ – Task 4 (Guo, Prendergast, Urban)

in situ XAS characterization at B K-edge under pressure of H$_2$ again reveals evidence of boron oxidation ... but also hydroxide (based on DFT interpretation).

TEY – surface sensitive
TFY – bulk sensitive
some oxidation may be helpful
reduced barriers for H$_2$ diss’n
Accomplishment: Synthesis and understanding of functional graphene nanoribbon Mg – Task 4,5 (Prendergast, Urban, Fischer)

Graphene Nano-Ribbons (GNR) synthesized by Fischer (LBNL)

Desorption at 300 ºC

Hydrogenation at 200 ºC, 15 bar

Atomically thin porous wrapper: selective physical barrier … explore additional chemical or catalytic functionality
Accomplishment: DFT simulations of interfacial structure of Mg/4N-GNR – Task 4,5 (Prendergast, Urban, Fischer)

Based on the thermodynamics, the edge of GNR may be terminated by H(-CH) or 2H(-CH₂) depending on the cycling conditions (temperature and pressure) and the substrate (Mg/MgH₂)

\[
G_H(\mu_H) = \frac{1}{2a} \left( E_{GNR} - E_{Mg} - \frac{N_o}{2} E_{\text{graphene}} - \frac{N_H}{2} E_{H_2} - N_H \mu_H - N_N \mu_N \right)
\]

\[
\mu_{H_2} = H^\circ(T) - H^\circ(0) - T S^\circ(T) + \frac{k_B T}{P} \ln \left( \frac{P}{P^\circ} \right)
\]

4N-GNR on Mg

4N-GNR on MgH₂

DFT Calculations: Wan, Prendergast, Synthesis: Urban and Fischer
Accomplishment: DFT simulations of interfacial structure of Mg/4N-GNR – Task 4,5 (Prendergast, Urban, Fischer)

vacancies drive $\text{H}_2$ dissociation

cold 4N-GNR

room temp

$\text{H}_2$

@Mg

induced vacancy

tailored *catalytic* function of atomically thin wrapper with enhanced thermodynamics and kinetics
Accomplishments: Synthesis of GNRs Functionalized with Binding Sites for Molecular Defined Hydrogen Dissociation Catalysts
– Task 5 (Fischer, Klebanoff)

- **Synthesis of GNRphen**
  1. Ni(COD)$_2$, bipy, COD, DMF, Tol, 80 °C, 3 d, 83%
  2. HClO$_4$, CH$_2$Cl$_2$, 0 °C, 2 h, 92%
  3. DDQ, THF, 45 °C, 2 d, 96%

- **Characterization of Transition Metal Complex Bound to GNRphen [phenRe(CO)$_3$]**

**Raman spectroscopy**

**IR spectroscopy**
Accomplishments: Coordination of a Potent Hydrogen Dissociation/Association Catalyst \([\text{phenIrCp}^*\text{OH}_2]\) to GNRphen

- **Task 5 (Fischer, Klebanoff)**

- **Challenge:** Modification of a Reported Synthesis of \([\text{phenIrCp}^*\text{OH}_2]\)

- **Accomplishment:** Preparation of \([\text{GNRphenIrCp}^*\text{OH}_2]\) catalyst to GNR active \(\text{H}_2\) dissociation catalyst (prepared as a reference)

![Chemical reaction diagram]

Continuing Work:

- Samples of \([\text{GNRphenIrCp}^*\text{OH}_2]\) and the parent complex \([\text{phenIrCp}^*\text{OH}_2]\) have been transferred to Sandia (L. Klebanoff) for \(\text{H}_2/\text{D}_2\) kinetic exchange studies.

- Integration of \([\text{GNRphenIrCp}^*\text{OH}_2]\) with hybrid \(\text{H}_2\) storage material (e.g \(\text{MgH}_2, \text{AlH}_3, \text{complex hydrides}\)) is ongoing.
Accomplishments: GCMC simulations of H₂ adsorption

- Tasks 1, 6 (Camp, Stavila, Prendergast, Haranczyk)

Simulation inputs:
1. Structures: MOF framework coordinates + H₂ geometry
2. Energetics: potentials for H₂–MOF and H₂–H₂ interactions
3. Equation of state:
   - Fugacity coefficients
   - Absolute adsorption → excess adsorption conversion

Simulation outputs:
*excess and absolute adsorption isotherms*

GCMC constant µ, V, T
variable number of H₂ adsorbates

Structures models from our Computation-Ready Experimental MOF database¹

H₂ potentials: 3-site and 5-site models that include dispersion and electrostatic interactions

NIST hydrogen equation of state² and Peng-Robinson equation of state compared to NIST reference data for H₂ densities and fugacities³

References:
Accomplishment (Sorbent thermodynamics): Library of MOFs for QMC and GCMC model validation

Predictions vs. Experiment (HyMARC)

77 K H$_2$ isotherms for canonical MOFs

⇒ GCMC calculations can be used to accurately predict the hydrogen adsorption isotherms and isosteric heats of adsorption in MOFs with and without open metal sites
Accomplishments: Simulations of H$_2$ adsorption in a model MOF-74

MOF-74 model system with variable number of active open metal site (OMS) atoms and OMS Lennard-Jones epsilon parameter (corresponding to the binding strength of OMS) was developed to seek the optimal values of these parameters that maximize H$_2$ deliverable capacities. Figure presents (each pixel correspond to one model structure):

(a) H$_2$ heat of adsorption at infinite dilution
(b) Deliverable capacity (pressure swing, constant temperature) between 100 bar and 5 bar at T = 77 K
(c) Deliverable capacity at T = 180 K
(d) Deliverable capacity at T = 243 K.

⇒ At 77 K, high interaction energy open metal sites are not needed to maximize H$_2$ deliverable capacity
⇒ At near-ambient temperatures (243 K), stronger OMS interaction energies increase deliverable capacity
⇒ At intermediate temperatures (180 K), there is an interesting tradeoff between these effects
Response to 2017 AMR Reviewer Comments

“Project Weaknesses”

- The diversity and number of ongoing efforts is a project weakness, but this is common with large and complex projects and should improve with time and the advent of more seedling projects. We used this feedback to sunset two projects that didn’t align with seedling research.

- Lack of characterization and analytical work on the Al-based hydride compared to the current Mg work. Related to above comment – we have focused our program on Mg-based materials such as MgB₂, Mg(BH₄)₂ to better align research goals across core labs and seedlings.

- The encapsulation effort did not appear to be laser-focused on providing an optimal model material platform for HyMARC collaborations, and it could benefit from better integrating with the HyMARC computational team’s needs. XAS results of encapsulated metal and pure metal have been supported by theoretical investigations to provide an optimal structure at the interface between metal and graphene. This collaborative work, published in Nano Letters (2017), provides a design strategy for property optimization using graphene-based materials.

- Unclear innovative synthetic strategies of light metal hydride in nanoscale via encapsulation. We have clarified which aspects of Mg(BH₄)₂ material properties, i.e. phase transition, reversibility.

- Experimental results leave important questions unaddressed. It is not clear what the nature of rGO coating is or why GO is used to modify water-sensitive Mg-borohydride when pristine oxygen-free graphene in an organic solvent would be a more appropriate option. We have proved theoretically that in Mg/rGO system, an atomically thin oxide layer at the interface between Mg nanoparticles and graphene encapsulation is beneficial for hydrogen storage applications. This is published in Nano Letter, 2017.
“Recommendations for additions/deletions to project scope”

- The project should perform similar encapsulation work and analysis to other metal hydrides to better understand the phenomena involved.

- The project should continue to investigate more complex metal hydrides.
  - We have been working on metal-doped magnesium hydrides and metal borohydride. We are addressing those works in this presentation. Metal-doped magnesium hydrides work is published in Advanced Energy Materials 2017
Collaborations

- HySCORE team (Long, UC Berkeley; Gennett, NREL)
- Godwin Severa, U of Hawaii (seedling project) – *molecular dynamics simulations of BH₄/etherate coordination of Mg*
- D.J. Liu, ANL (seedling project) – *initial discussions of X-ray spectroscopic characterization of NaBH₄ NPs in graphene and exploration of borohydride-graphene interactions*
- Agiltron, Inc. Scale up of encapsulated metal hydrides via SBIR
Remaining Challenges and Barriers

- Achieve size control in synthesis of encapsulated Mg(BH$_4$)$_2$ materials
- Incorporate theoretical insights on graphene-hydride interface into advanced synthesis of these materials
- Performing in-situ soft x-ray spectroscopies achieving realistic hydrogen storage (i.e. UHV requirement)
- Understanding coordination/reactivity of Mg(BH$_4$)$_2$ with oxide and graphene interfaces
- Standard GCMC simulation approaches for prediction of H$_2$ adsorption involve transferable force-fields which do not sufficiently describe specific MOFs with open metal sites
- The relations between the strength and number of open metal sites, overall pore morphology and the adsorbent performance in H$_2$ storage are not fully understood
Proposed Future Work

• Further develop *in-situ* XAS cell for operating at higher temperatures (600° C) and higher H₂ pressure (up to 10 bar) required focused X-ray beam
• Determination of the phase transition in Mg(BH₄)₂ NPs wrapped by rGO by *in-situ* XAS and simulations – Task 1,4
• Kinetic study of H₂/D₂ exchange with [GNRphenIrCp*OH₂] as a model for hydrogen activation. Comparison of the performance of GNR conjugated catalysts to the parent molecular structure – Task 5
• Synthesis of hybrid system composed of nanodispersed hydrogen storage material (e.g MgH₂, AlH₃, complex hydrides) encapsulated in a [GNRphenIrCp*OH₂] matrix. Evaluation of the hydrogen absorption/desorption kinetics - Task 4
• Development of a protocol to perform simulations of hydrogen adsorption in MOFs without empirical parameters (ab initio isotherms). Characterization of large sets of materials – Task 1,6
• Systematic study of the relation between the structure and chemistry of diverse MOFs, and H₂ adsorption (so far, we have done it only for an example 1D channel system based on MOF74) – Task 1,6

Any proposed future work is subject to change based on funding levels.
Technology Transfer Activities

- Agiltron, Inc. together with Urban won a Phase 2 SBIR relating to scale up and kinetics of encapsulated metal hydrides
- HyMARC presented research at annual Tech Team meeting
- 2 new patents, and 3 new records of invention filed in the past year.

Any proposed future work is subject to change based on funding levels.
Summary

- Synthetic-control over various phases of Mg(BH$_4$)$_2$ NPs in rGO with the reversibility
- Development of *in-situ* H$_2$ XAS capability at ALS for absorption/desorption experiments
- *In-situ* XAS measurements of Mg(BH$_4$)$_2$ up to H$_2$ pressure of 1 bar
- Synthesis of carbon based matrix containing phen binding sites for molecular defend H$_2$ activation catalysts.
- Synthesis and IR/Raman characterization of a highly active H$_2$ dissociation catalyst [GNRphenIrCp*OH$_2$] bound to a GNRphen matrix.
- Demonstrated ability to model high-pressure H$_2$ storage in metal-organic framework adsorbents using classical GCMC, and verified the simulations using experiments run within HyMARC
<table>
<thead>
<tr>
<th>Project Milestone</th>
<th>Type</th>
<th>Task Completion Date</th>
<th>Progress Notes</th>
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<tbody>
<tr>
<td>Use QMC, DFT, and force fields to compute H₂ binding and select appropriate levels of theory for MOFs.</td>
<td>PM</td>
<td>12/31/17 - 3/31/18 - 70%</td>
<td>LLNL and LBNL are working on finite-size/extended system corrections based on MOF-74. Study of different DFT functionals on model noncovalent systems published in recent sorbent review.</td>
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<tr>
<td><strong>Revised milestone</strong>: Compute H₂ binding curves with different computational methods for model MOFs to establish protocol for accurate physisorption calculations</td>
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<tr>
<td>Sensitivity analysis of local binding and second-sphere effects</td>
<td>PM</td>
<td>3/31/17 - 9/30/17 - 100%</td>
<td>Completed by Maciek Haranczyk (LBNL) for open metal sites in MOFs. Results to appear in sorbent perspective.</td>
</tr>
<tr>
<td>Rank improvement strategies for sorbents. Decision criterion: select 2 with greatest potential for increasing ΔH°</td>
<td>GNG</td>
<td>3/31/17 - 3/31/17 - 100%</td>
<td>Strategy and results reported at AMR. Manuscript for submission to En. Env. Sci. in progress.</td>
</tr>
<tr>
<td>Modify LEIS instrument to enable laser-induced thermal desorption</td>
<td>PM</td>
<td>6/30/17 - 6/30/17 - 100%</td>
<td>Demonstrated feasibility of ion beam-based desorption technique</td>
</tr>
<tr>
<td>Evaluate additive/composite strategies for improving effective ΔE</td>
<td>PM</td>
<td>9/30/17 - 9/30/18 - 75%</td>
<td>Evaluation of multiple strategies in progress.</td>
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</table>

PM=progress measures; M=SMART milestone; GNG=Go/No-go.
<table>
<thead>
<tr>
<th>Planned Milestones and Status: FY17 and FY18</th>
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<tbody>
<tr>
<td><strong>Prototype hydride surface and interface chemistry kinetic models</strong></td>
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<tr>
<td><strong>Amorphous phases and defects model formalism</strong></td>
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<tr>
<td><strong>Sensitivity analysis of morphology and microstructure</strong></td>
</tr>
<tr>
<td>Completed analysis, reported in LLNL AMR slides</td>
</tr>
<tr>
<td>Rank improvement strategies for hydrides. Decision criterion: select 2 with greatest potential for reducing effective $\Delta H$</td>
</tr>
<tr>
<td>Parameterize integrated kinetic model for representative B-N-Al-hydrides</td>
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<tr>
<td>Compute sorbent isotherms from QMC data using CoRE database of MOFs</td>
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<tr>
<td>Milestone delayed until Phase 2 due to lack of personnel with requisite expertise</td>
</tr>
<tr>
<td>Public release of codes, databases, synthetic protocols, characterization methodologies optimized for storage materials</td>
</tr>
<tr>
<td>Revised language: Public release of databases, synthetic protocols, characterization methodologies optimized for storage materials</td>
</tr>
</tbody>
</table>

PM=progress measures; M=SMART milestone; GNG=Go/No-go.
HyMARC Collaboration and Funding Partners

Enabling **twice the energy density** for onboard H₂ storage
Technical Back-Up Slides
Challenge: Incorporation of Discrete Hydrogen Dissociation Catalysts into the Shell of GNR Encapsulated Hydride Storage Materials

Scientific Question:
- Can we lower the reversible H\textsubscript{2} dissociation/association activation barrier by introducing known discrete homogeneous hydrogen dissociation catalysts in the nanoparticle matrix?

Technical Challenge:
- Can we decorate the edges of graphene nanoribbons (GNRs) with metal coordination sites that co-locate the H\textsubscript{2} dissociation/association catalysts at the GNR nanoparticle interface?
Remaining challenges and future plans for soft x-ray spectroscopies @ ALS (Guo)

Performing in-situ soft x-ray spectroscopies achieving realistic hydrogen storage are extremely challenging (i.e. UHV requirement)

Future instrumentation developments planning to overcome challenges

**In-situ cells**
(high T >600°C & P >10bars)

- New cell designs
- High-pressure x-ray transparent membrane development
  (smaller in size, requires focused x-ray beam)

**In-situ XAS & RIXS Beamlines**

- Beamline 8.0.1.4 (in operation) 80-1250 eV
  *Commissioning soon*
- Beamline 7.3.1 (August 2018) 250-2000 eV
- Beamline 6.0.1 (Spring 2019) 250-2500 eV

**Burst pressure vs. membrane size**

- B K-edge 200 eV
- N K-edge 400 eV
- T.M. L-edges 400-1100 eV
- Na, Mg, Al & Si K-edge <2500 eV