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

HyMARC Hydrogen Materials Advanced Research Consortium

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

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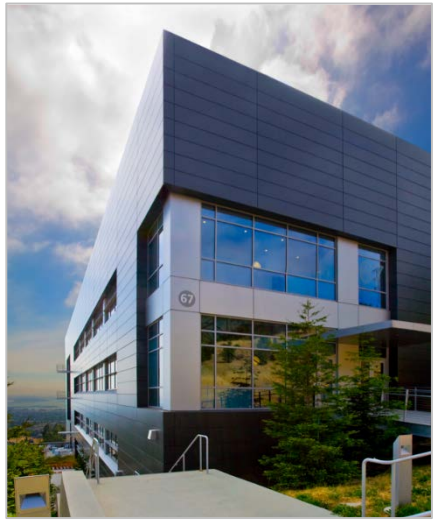
Berkeley, California USA

BERKELEY LAB

2018 DOE Hydrogen Annual Merit Review
June 7, 2018

Project ST130



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Overview (LBNL)

Timeline

Project start date: 09/21/2015
Phase I end date: 09/30/2018

Barriers addressed

- Lack of understanding of hydrogen physisorption and chemisorption (Barrier O)
- System weight and volume (Barrier A)
- Charge/discharge rate (Barrier E)

Budget

FY17 DOE Funding: $770K
FY18 DOE Funding: $775K
Total Funds Received: $2.585M (all years)

Team

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

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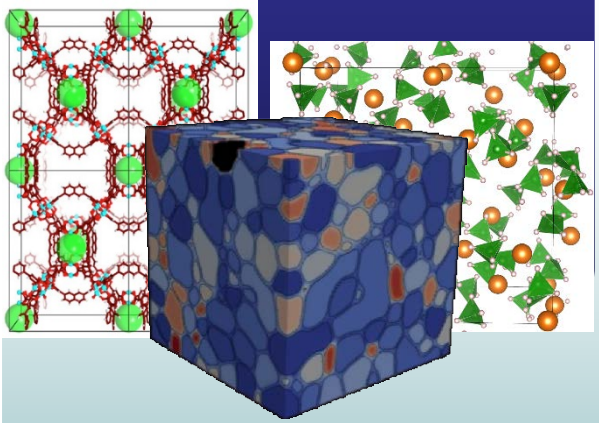
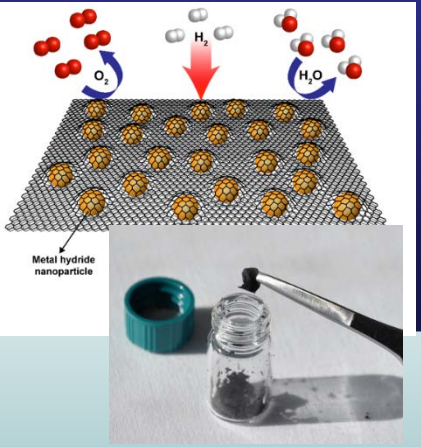
Theory, simulation, & data



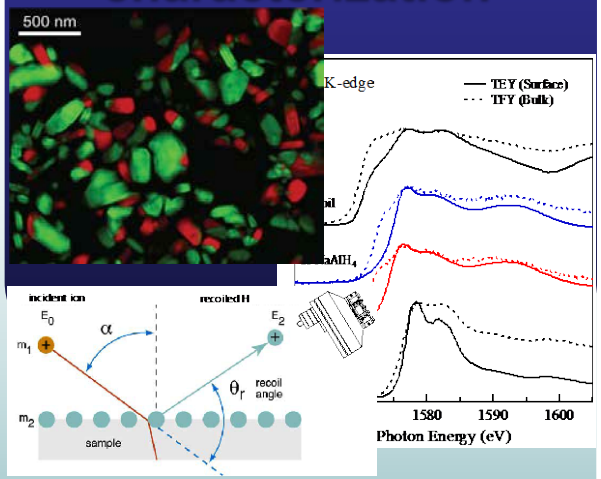
- Quantum Monte Carlo for sorbents
- **DFT and *ab initio* molecular dynamics for bulk/surface/interface chemistry**
- Classical MD & kinetic Monte Carlo for non-equilibrium transport
- Phase-field modeling for solid-state phase transformation kinetics
- **Computational spectroscopy**
- **Community software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

Relevance (LBNL-specific): Materials by Design Coupled with Advanced Characterization and Modeling

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 H_2 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

Tasks	LBNL Team:
2,3,4,5	**Jinghua Guo** (jguo@lbl.gov): X-ray synchrotron spectroscopy
2,3,4,5	**David Prendergast** (dgprendergast@lbl.gov): Computational spectroscopy
1,4	**Jeff Urban** (jjurban@lbl.gov): Phase transitions and nanoscale effects in hydrides
1,5	**Gabor Somorjai** (gasomorjai@lbl.gov): Functional sorbents
1	**Felix Fischer** (ffischer@lbl.gov): Functionalized graphene nanoribbons
6	**Maciek Haranczyk** (mharanczyk@lbl.gov): Materials genome for porous materials

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):

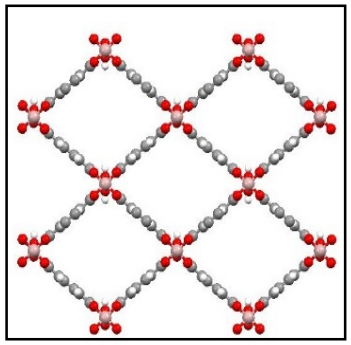
- Soft X-ray absorption/emission spectroscopies (XAS/XES) – in situ
- Ambient Pressure XPS
- Scanning Transmission X-ray Microscopy (STXM) and Ptychography

Active user projects at TMF and ALS and Approved Program Proposal @ ALS

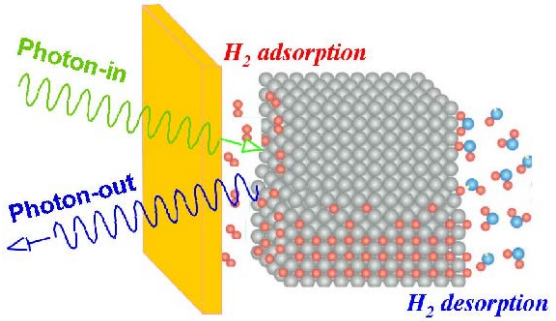
- partnership to foster a new soft X-ray H_2 storage user community

Technical Approach: Matched Novel Synthesis, Characterization, and Modeling for Storage Materials

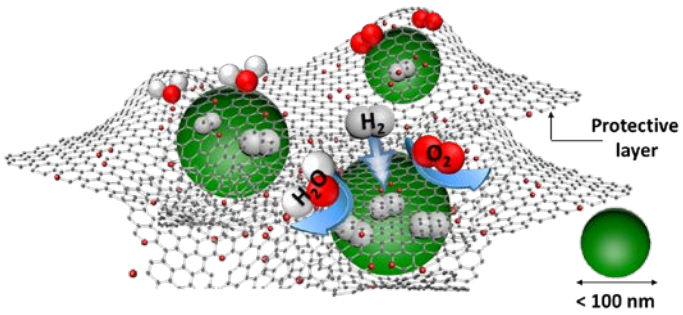
Theory & Design of Storage Materials



Characterization

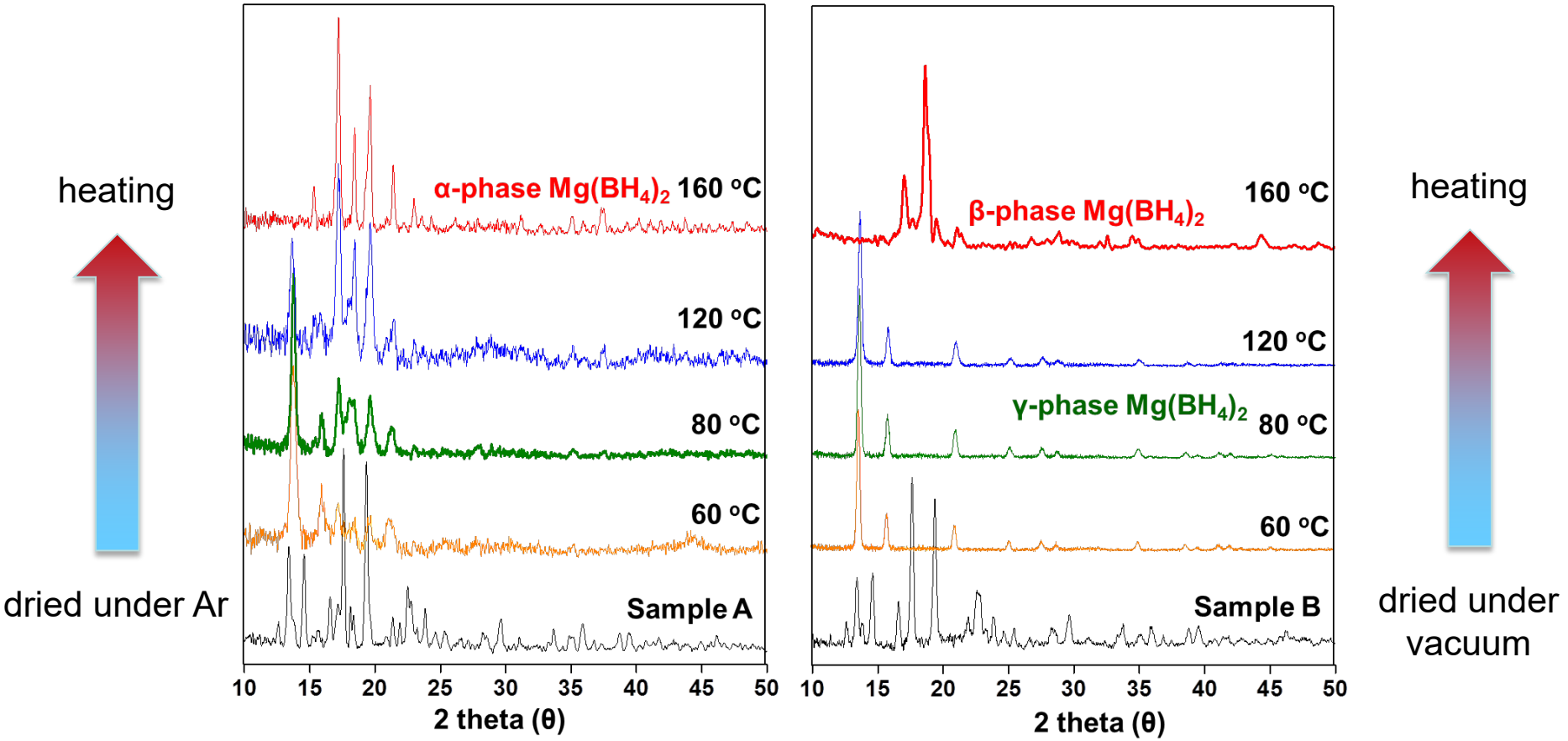


Synthesis & Performance Evaluation



- 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 H_2 release/absorption and motivate new H_2 storage materials
- Developing new acid/base concepts to modify the enthalpy of H_2 binding in sorbents
- Creating algorithms to enable computation of H_2 isotherms in framework materials
- *In-situ* spectroscopic and structural characterization techniques that establish the role of interfaces in controlling H_2-storage reaction mechanisms and pathways;
- Computational modeling of structure, chemistry and dynamics of interfaces and additives for nanoscale H_2 storage systems and interpretation of X-ray spectroscopy

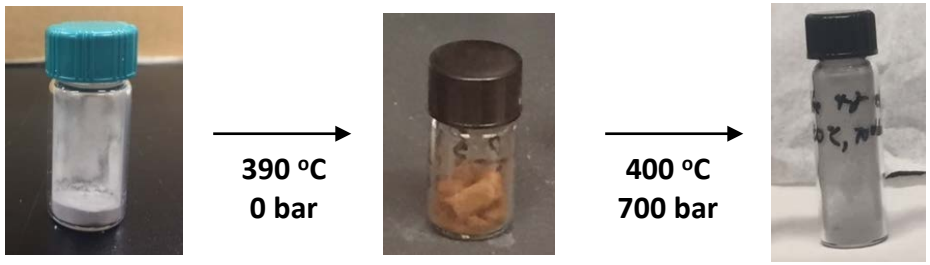
Accomplishment: Synthetic control over $Mg(BH_4)_2$ nanoparticle phase - *Tasks 1,4 (Urban)*



- First achievement of the pure phase control in encapsulated $Mg(BH_4)_2$/rGO materials
- Development of the facile synthetic method for 3 different phases (alpha, beta, gamma) of $Mg(BH_4)_2$

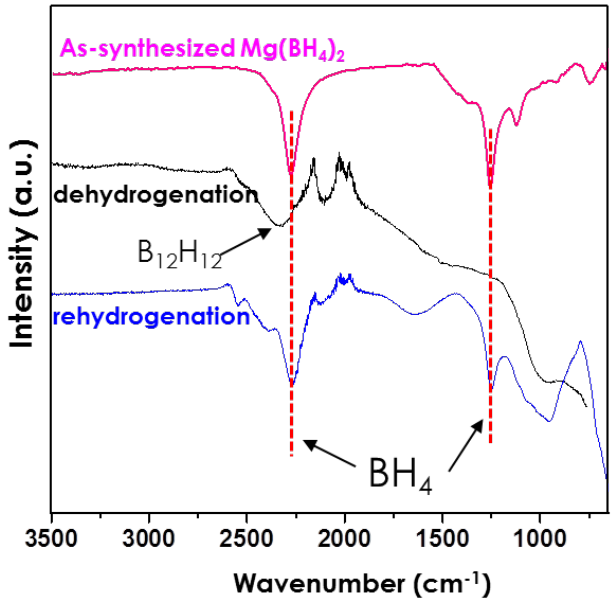
Accomplishment: Reversibility in γ-$Mg(BH_4)_2$/rGO – *Tasks 2,3,4 (Urban)*

i. $Mg(BH_4)_2$/rGO(MBHg) ii. Dehydrogenated MBHg iii. Rehydrogenated MBHg

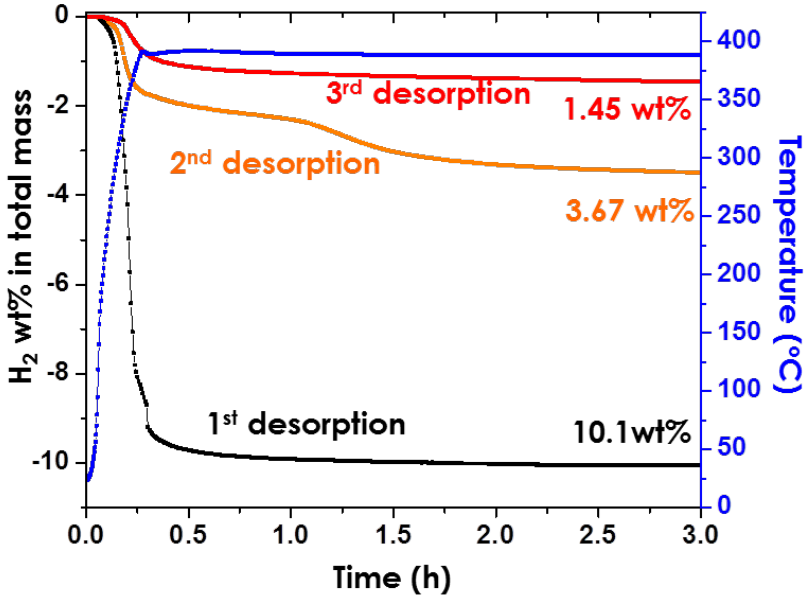


(collaborative with J. White and V. Stavila from Sandia)

FT-IR



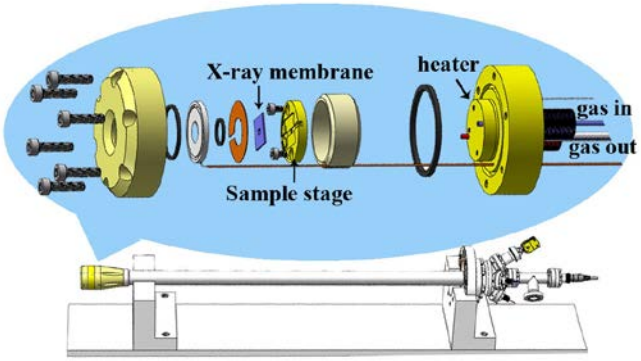
H_2 uptake isotherm



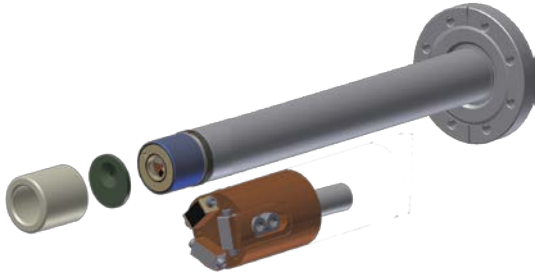
Our $Mg(BH_4)_2$/rGO hybrids also show reversibility for alpha/beta phases - not demonstrated in literature

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)



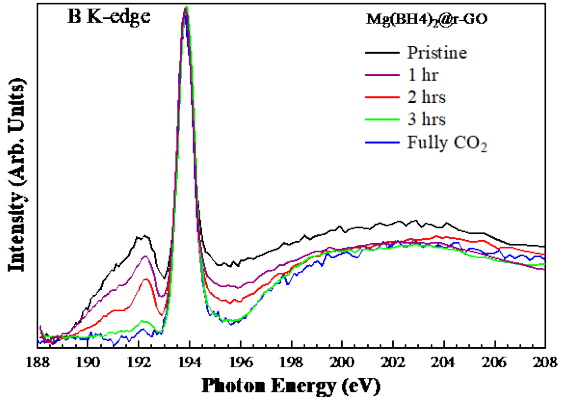
In-situ flow gas cell (1 bar, max. 250˚C)



- 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.

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

- Material based H_2 absorption/desorption and CO_2 capture can be studied using in-situ/quasi XAS technique.



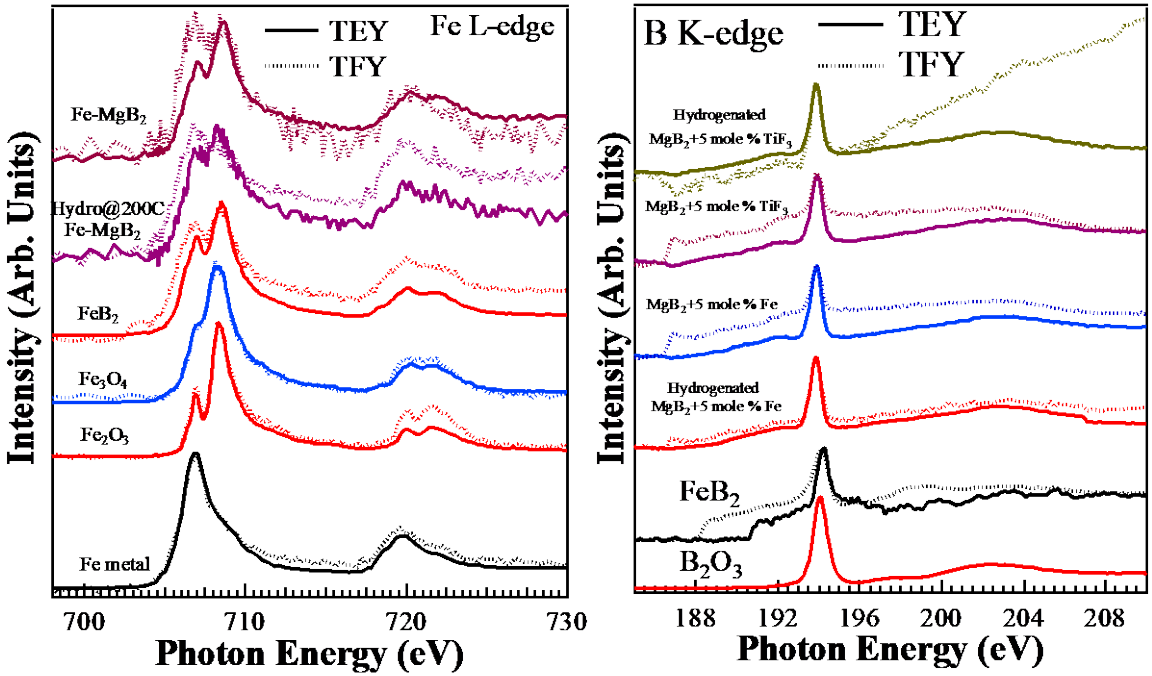
- Proposed experiments in progress from Urban's Group. ($Mg(BH_4)_2$)

Y.-S. Liu et al., *in preperation*

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)

Fe or TiF_3 doped MgB_2



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)*

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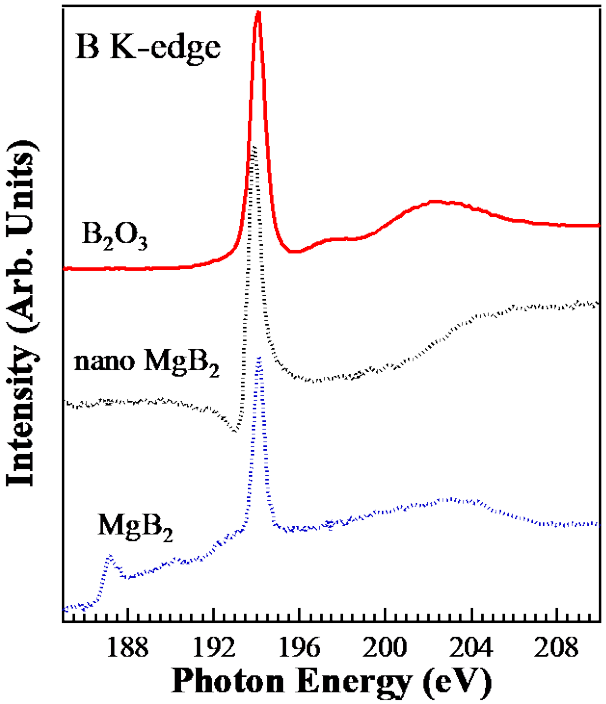
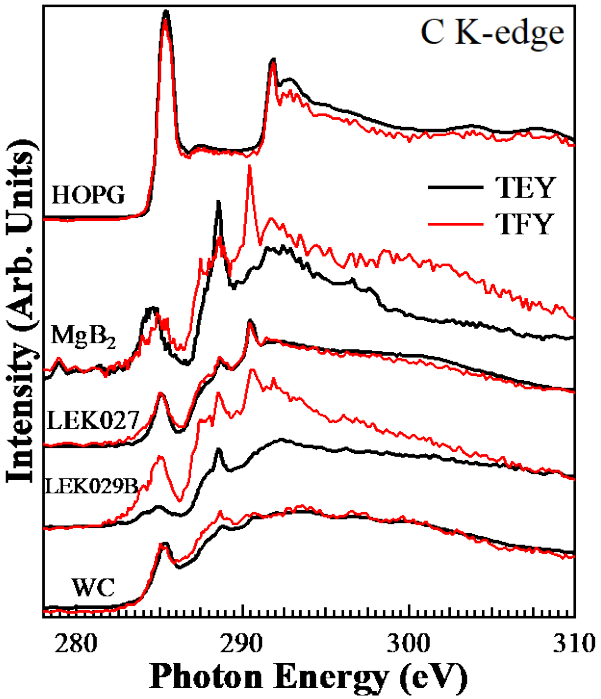
Nano MgB_2



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)*

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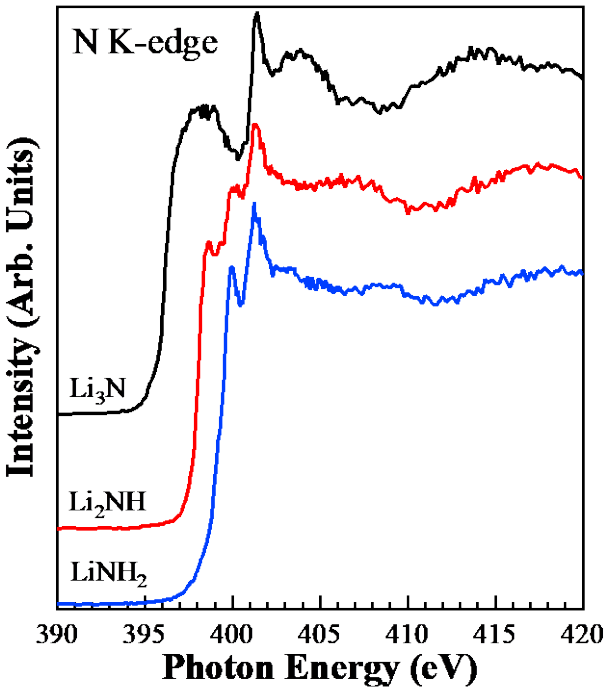
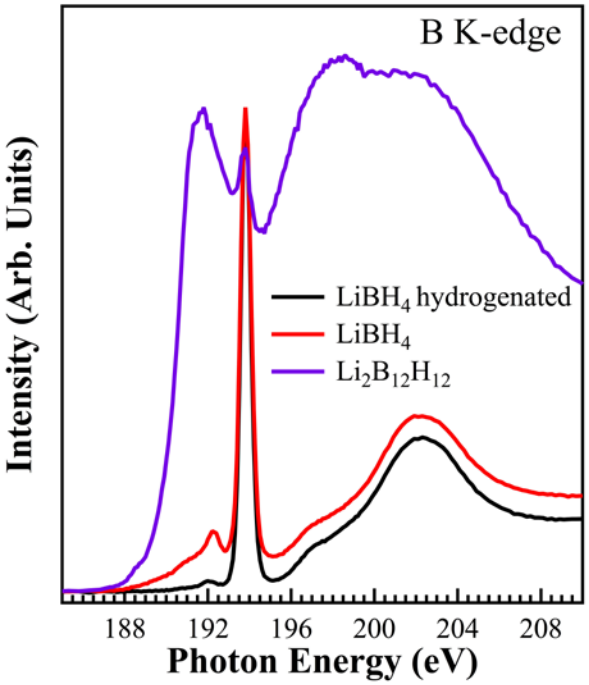
Lithium nitride



Lithium borohydride



TEY – surface sensitive
TFY – bulk sensitive

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

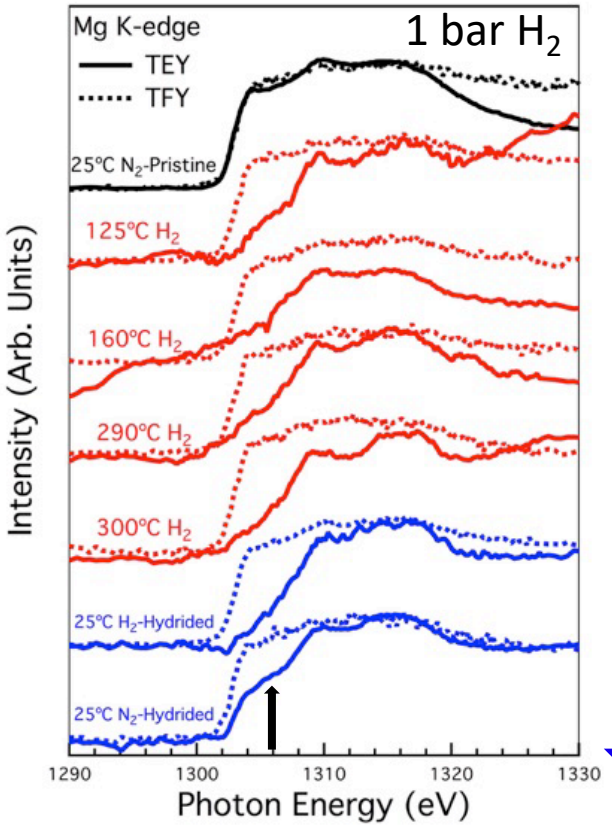
B oxidation ever present

K. G. Ray et al., *Phys. Chem. Chem. Phys.*, 2017

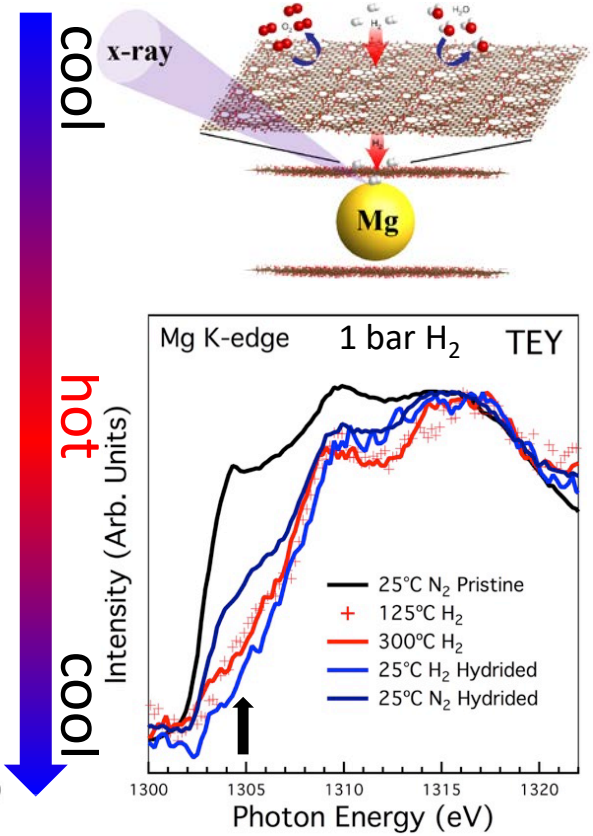
L. E. Klebanoff et al, *in preparation*

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

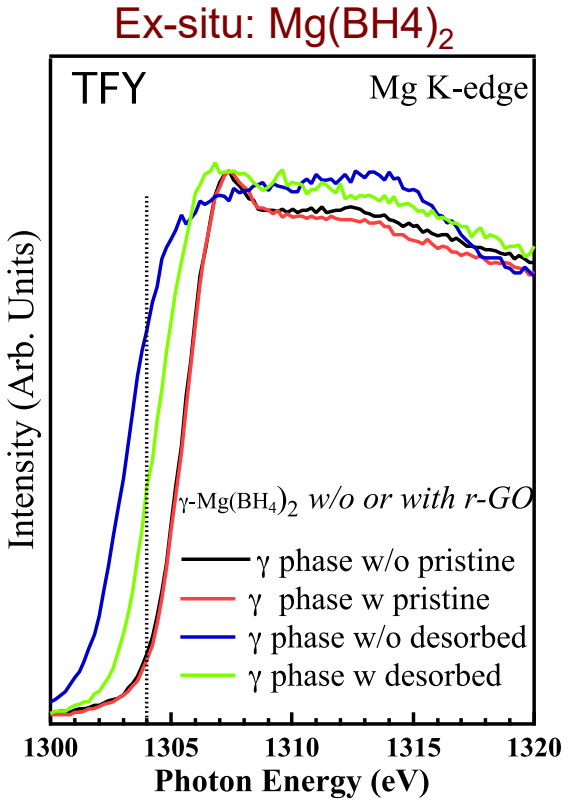
- Ni-doped rGO-Mg shows enhanced kinetic, the in-situ XAS characterization showing Mg hydride detected at 1 bar H_2 environment.



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)



First XPS study of $Mg(BH_4)_2$ to our knowledge

S. Jeong et al., in prep.

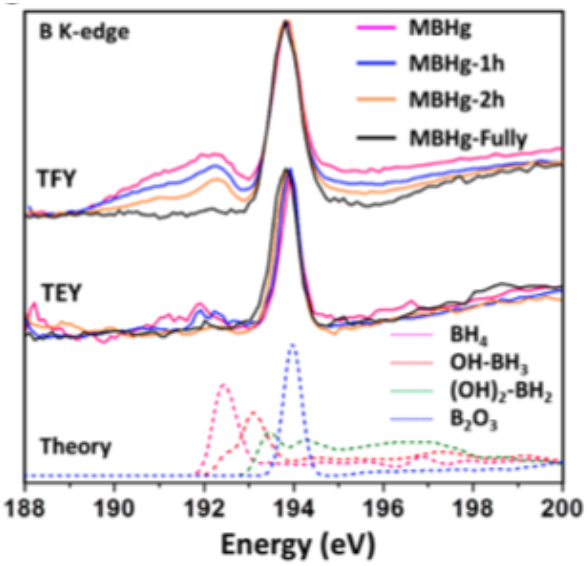
Accomplishment: In situ characterization on $Mg(BH_4)_2$ – *Task 4 (Guo, Prendergast, Urban)*

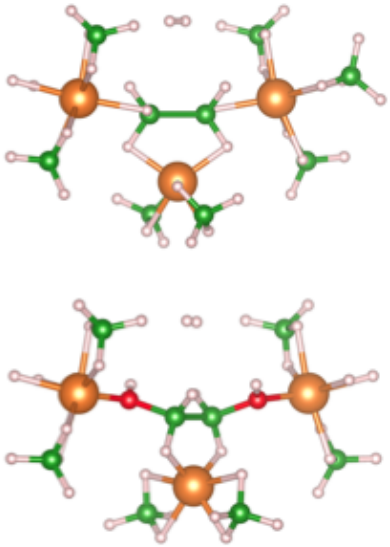
in situ XAS characterization at B K-edge under pressure of H_2 again reveals evidence of boron oxidation … but also hydroxide (based on DFT interpretation).

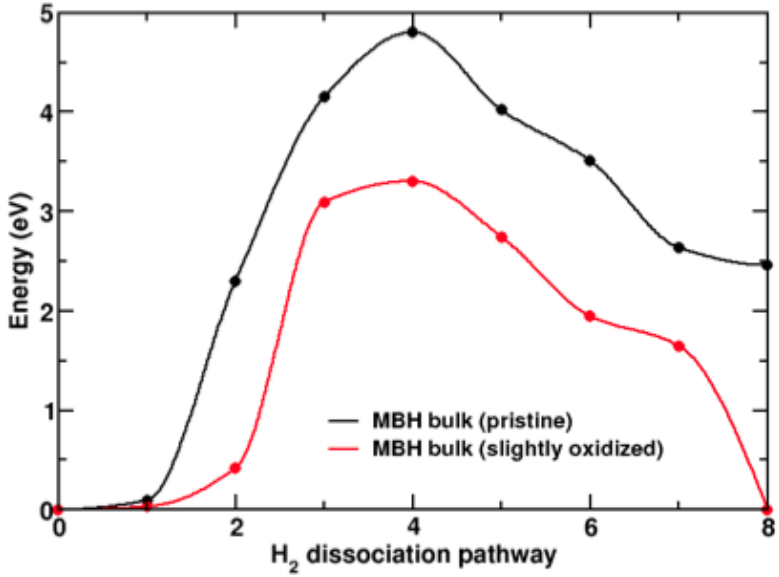
TEY – surface sensitive
TFY – bulk sensitive

some oxidation may be helpful

reduced barriers for H_2 diss'n

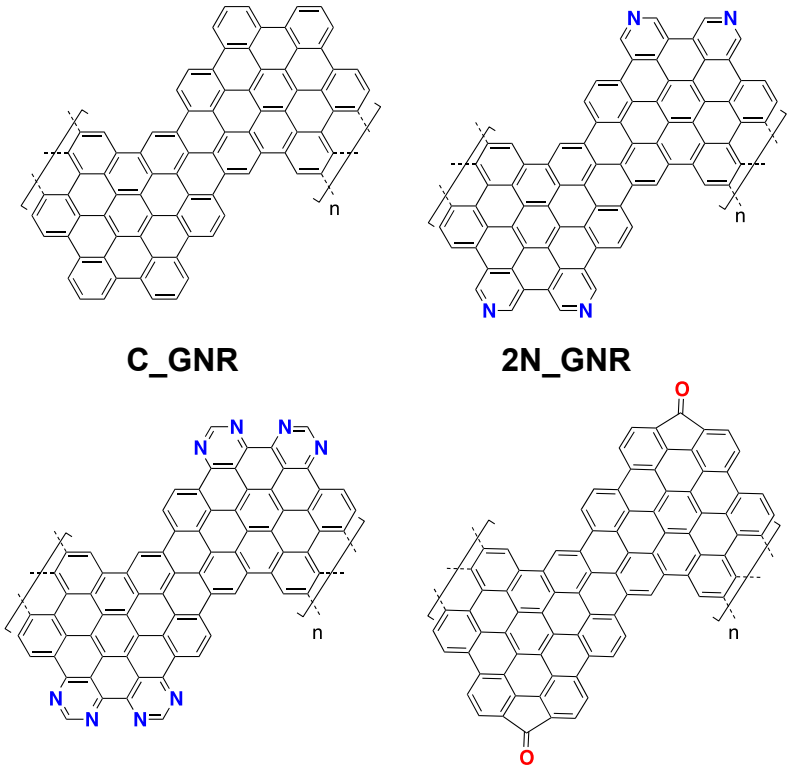


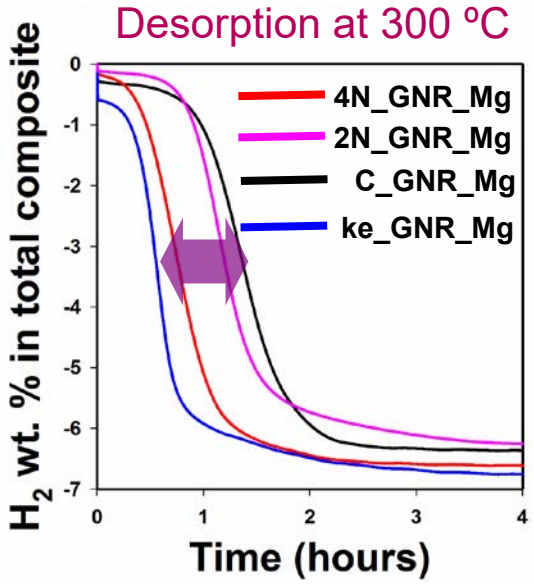


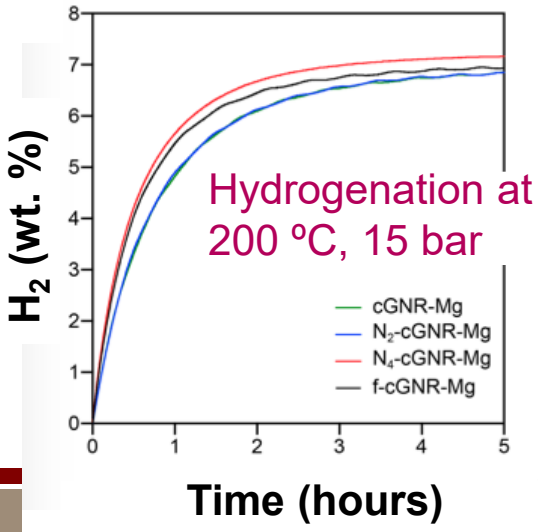


Accomplishment: Synthesis and understanding of functional graphene nanoribbon Mg – *Task 4,5 (Prendergast, Urban, Fischer)*

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







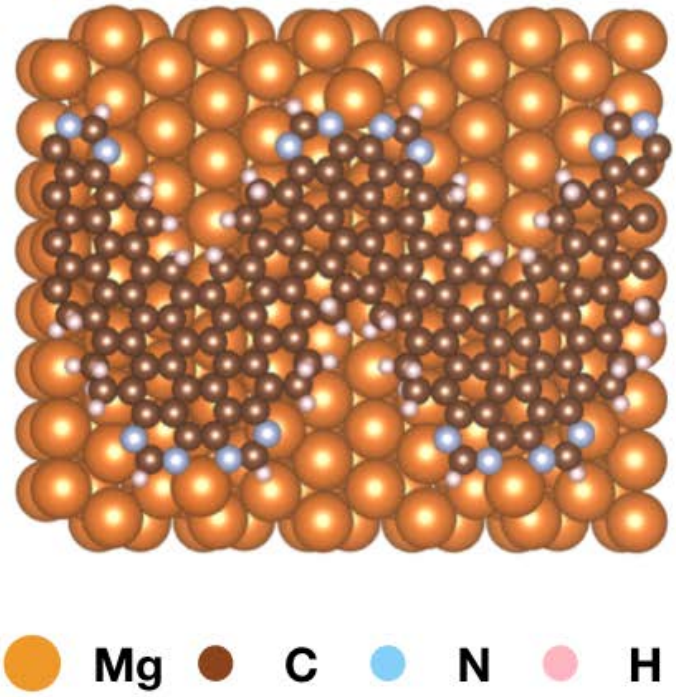
Atomically thin porous wrapper: selective physical barrier
… explore additional ***chemical*** or ***catalytic*** functionality

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

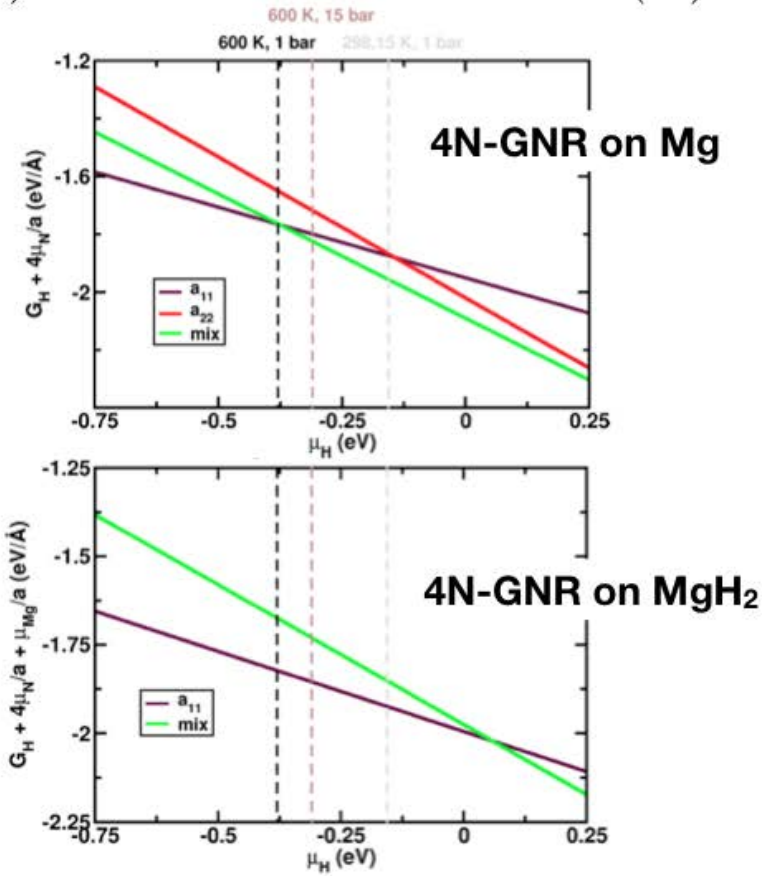
Based on the thermodynamics, the edge of GNR may be terminated by H(-CH) or 2H(-CH_2) depending on the cycling conditions (temperature and pressure) and the substrate (Mg/MgH_2)

$$G_H(\mu_H) = \frac{1}{2a}\left(E_{GNR} - E_{Mg} - \frac{N_c}{2}E_{graphene} - \frac{N_H}{2}E_{H_2} - N_H\mu_H - N_N\mu_N\right)$$

$$\mu_{H_2} = H^\circ(T) - H^\circ(0) - TS^\circ(T) + k_BT\ln\left(\frac{P}{P^\circ}\right)$$

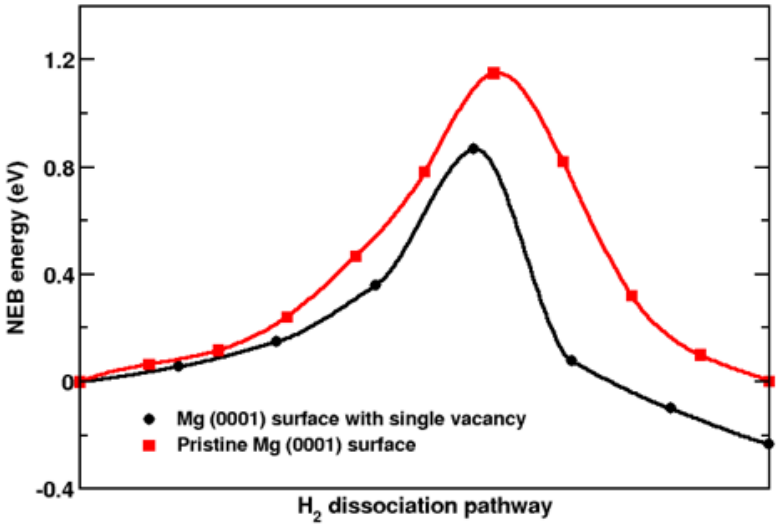


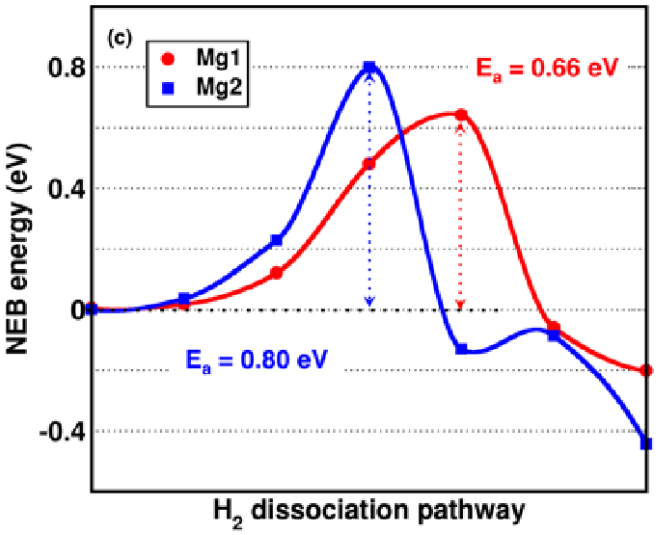
DFT Calculations: Wan, Prendergast, Synthesis: Urban and Fischer

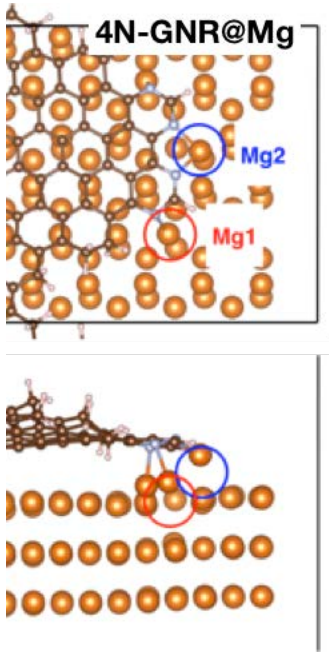


Accomplishment: DFT simulations of interfacial structure of Mg/4N-GNR – *Task 4,5 (Prendergast, Urban, Fischer)*

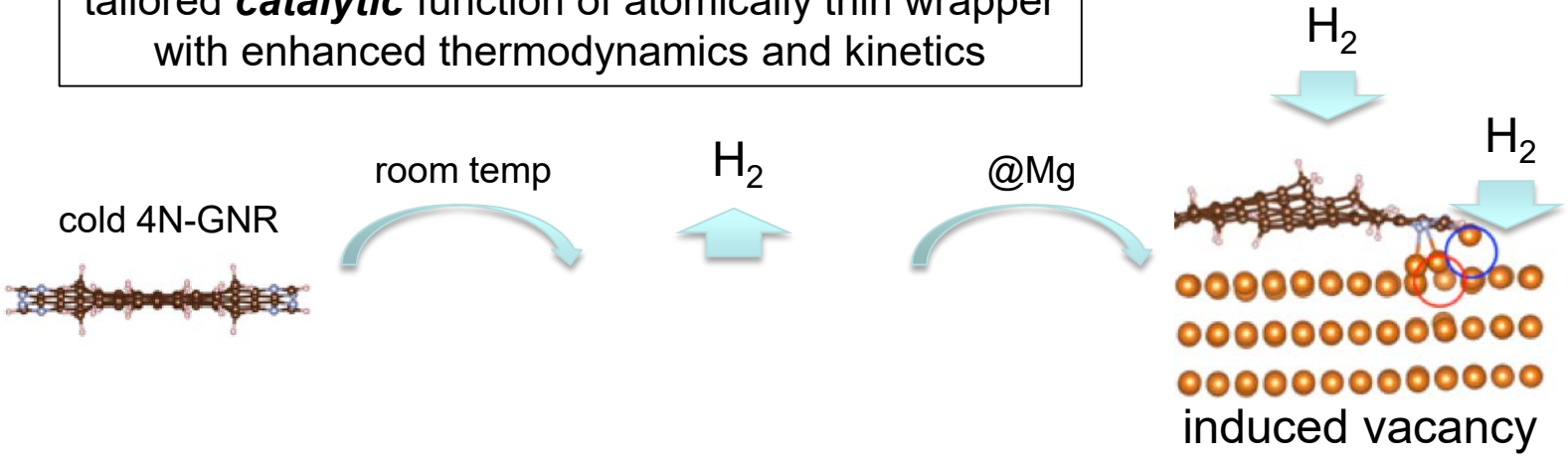
vacancies drive H_2 dissociation





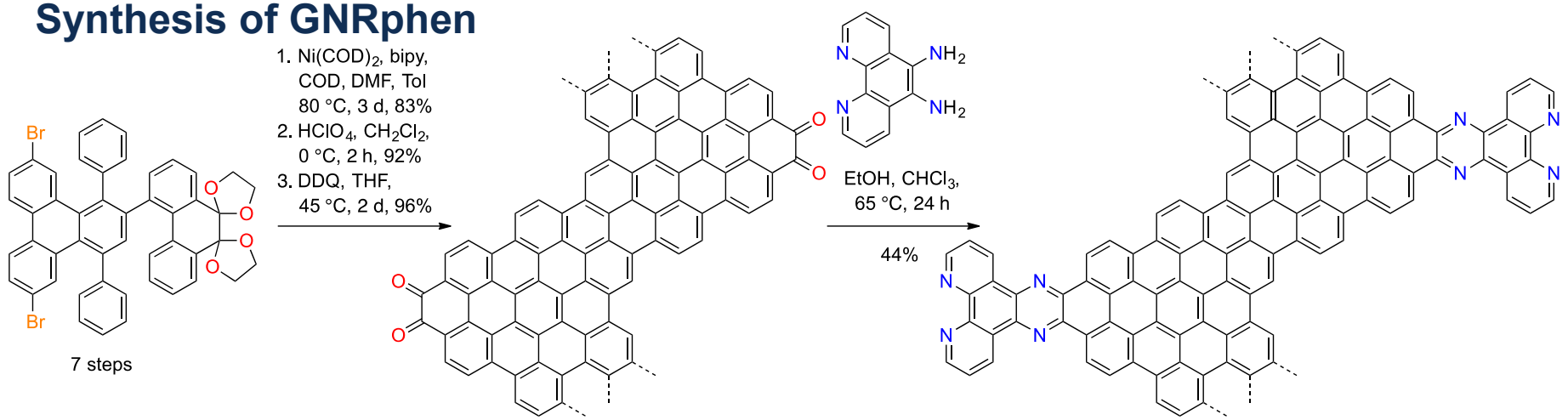


tailored ***catalytic*** function of atomically thin wrapper with enhanced thermodynamics and kinetics



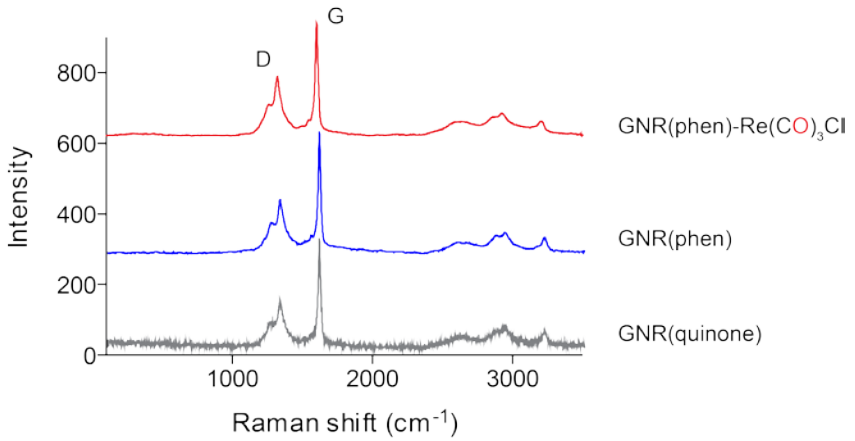
Accomplishments: Synthesis of GNRs Functionalized with Binding Sites for Molecular Defined Hydrogen Dissociation Catalysts – *Task 5 (Fischer, Klebanoff)*

- **Synthesis of GNRphen**

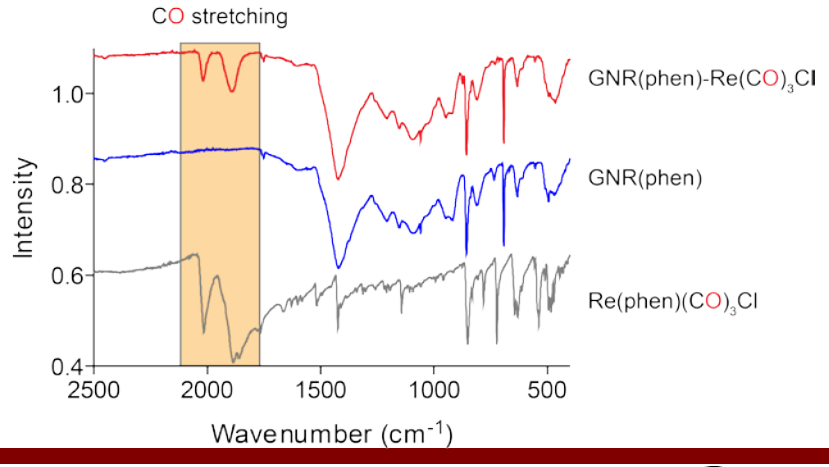


- **Characterization of Transition Metal Complex Bound to GNRphen [phenRe(CO)$_3$]**

Raman spectroscopy

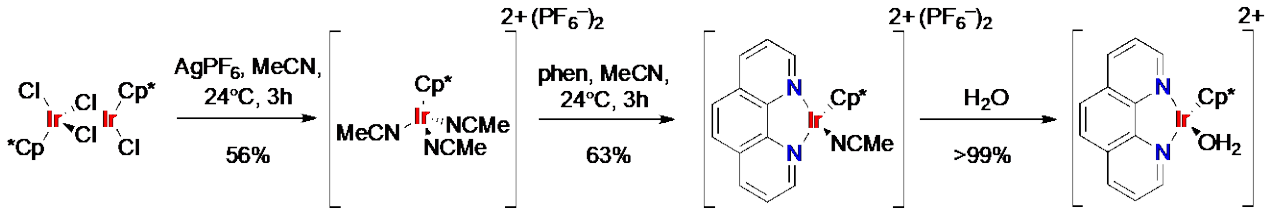


IR spectroscopy



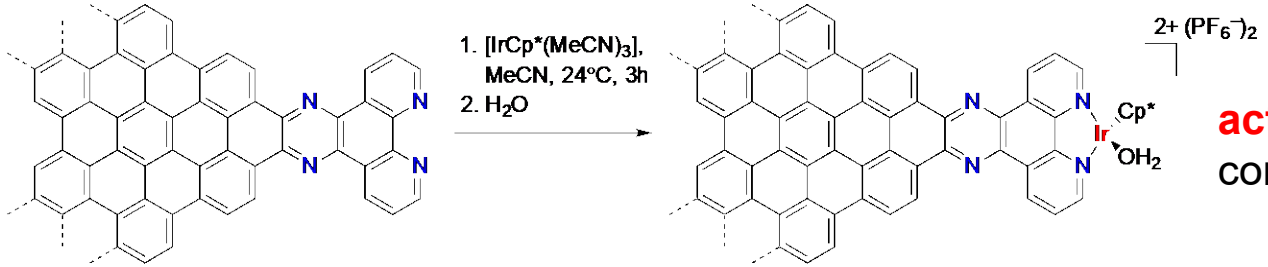
Accomplishments: Coordination of a Potent Hydrogen Dissociation/Association Catalyst [phenIrCp*OH_2] to GNRphen – *Task 5 (Fischer, Klebanoff)*

- **Challenge: Modification of a Reported Synthesis of [phenIrCp*OH_2]**



active H_2 dissociation catalyst (prepared as a reference)

- **Accomplishment: Preparation of [GNRphenIrCp*OH_2] catalyst to GNR**

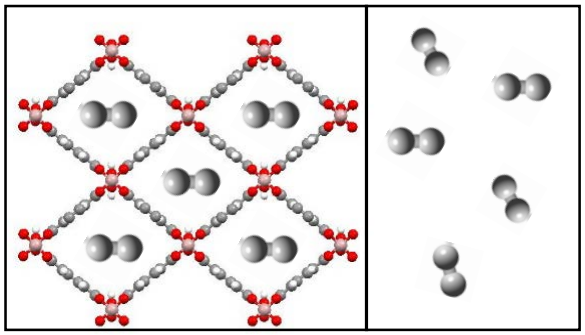


active H_2 dissociation catalyst conjugated to carbon matrix

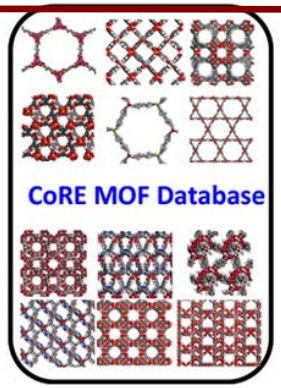
Continuing Work:

- Samples of [GNRphenIrCp*OH_2] and the parent complex [phenIrCp*OH_2] have been transferred to Sandia (L. Klebanoff) for H_2/D_2 kinetic exchange studies.
- Integration of [GNRphenIrCp*OH_2] with hybrid H_2 storage material (e.g MgH_2, AlH_3, complex hydrides) is ongoing.

Accomplishments: GCMC simulations of H_2 adsorption
-Tasks 1, 6 (Camp, Stavila, Prendergast, Haranczyk)



GCMC
constant μ,V,T
variable number of
H_2 adsorbates



Simulation inputs:

1. Structures: MOF framework coordinates + H_2 geometry
2. Energetics: potentials for H_2 – MOF and H_2– H_2 interactions
3. Equation of state:
   - Fugacity coefficients
   - Absolute adsorption → excess adsorption conversion

Simulation outputs:
excess and absolute adsorption isotherms

Structures models from our Computation-Ready Experimental MOF database[1]

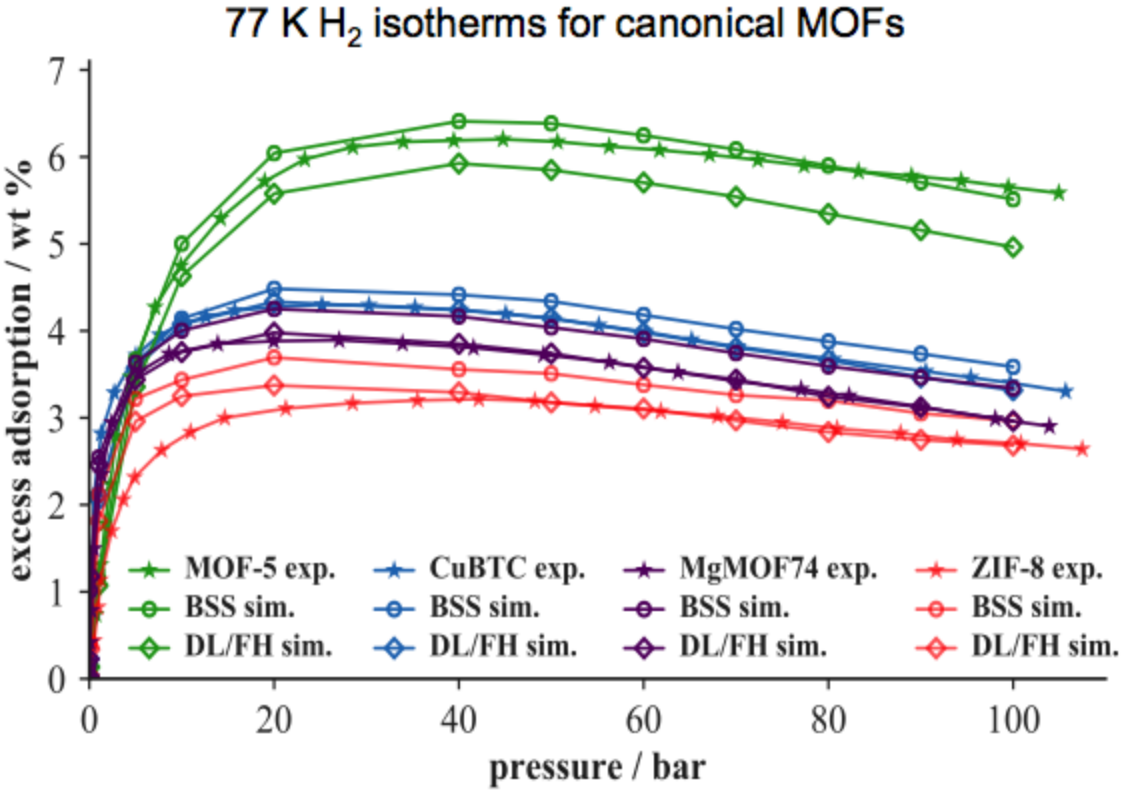
H_2 potentials: 3-site and 5-site models that include dispersion and electrostatic interactions

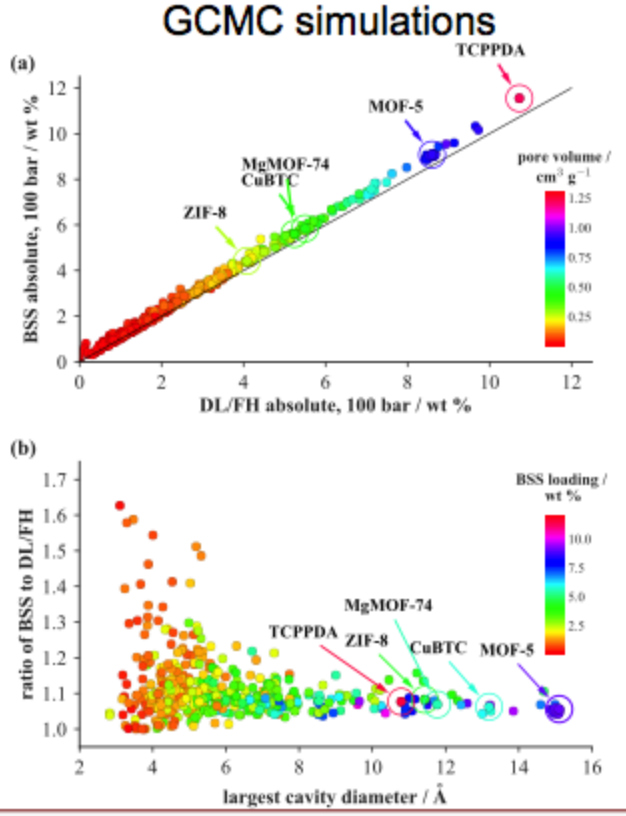
NIST hydrogen equation of state[2] and Peng-Robinson equation of state compared to NIST reference data for H_2 densities and fugacities[3]

1. Chung, Y. G.; Camp, J.; Haranczyk, M. et al., Computation-ready, experimental metal-organic frameworks: A tool to enable high-throughput screening of nanoporous crystals. *Chemistry of Materials* **2014**, *26*, 6185-6192.
2. Lemmon, E. W.; Huber, M. L.; Leachman, J. W., Revised standardized equation for hydrogen gas densities for fuel consumption applications. Journal of Research of the National Institute of Standards and Technology **2008**, *113*, 341.
3. Zhou, L.; Zhou, Y., Determination of compressibility factor and fugacity coefficient of hydrogen in studies of adsorptive storage. Int J Hydrogen Energ **2001**, *26*, 597-601.

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

Predictions vs. Experiment (HyMARC)





⇒ ***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***

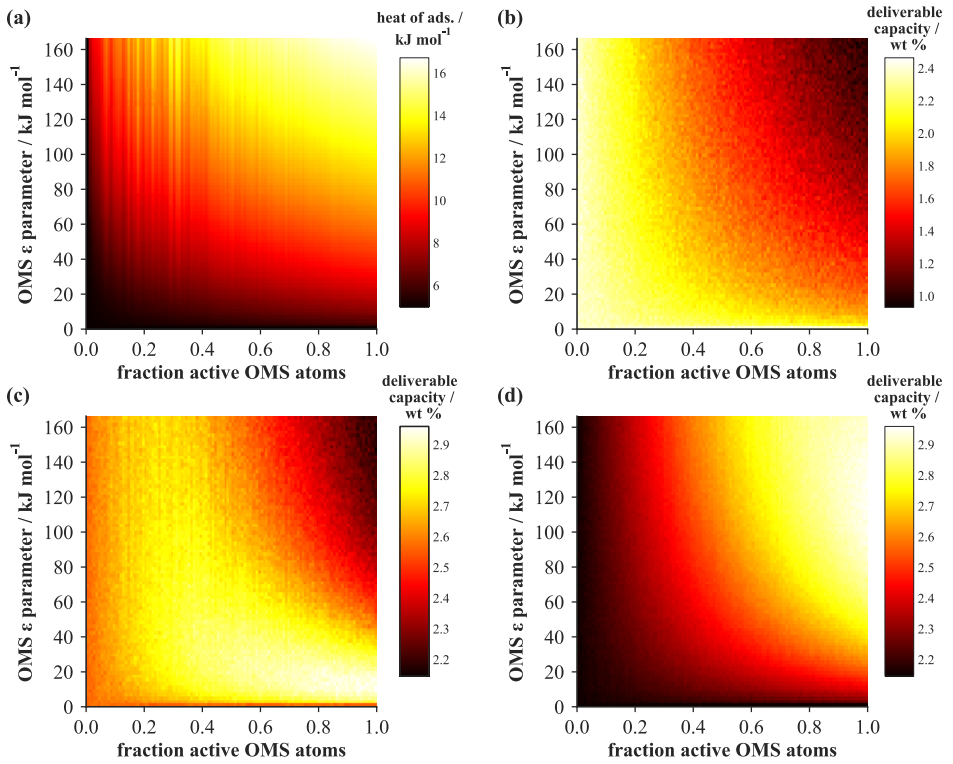
James White
Vitalie Stavila
Mark Allendorf

Aurora Pribram-Jones
Keith Ray
Brandon Wood

Jeff Camp
Maciek Haranczyk
David Prendergast

Katie Hurst
Philip Parilla
Tom Gennett

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 H2 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 MgB_2, $Mg(BH_4)_2$ 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 $Mg(BH_4)_2$ 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.

Response to 2017 AMR Reviewer Comments

"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 BH_4/etherate coordination of Mg*
- D.J. Liu, ANL (seedling project) – *initial discussions of X-ray spectroscopic characterization of $NaBH_4$ 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^{o} C) and higher H_2 pressure (up to 10 bar) required focused X-ray beam
- Determination of the phase transition in $Mg(BH_4)_2$ NPs wrapped by rGO by in-situ XAS and simulations – Task 1,4
- Kinetic study of H_2/D_2 exchange with [GNRphenIrCp*OH_2] 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 MgH_2, AlH_3, complex hydrides) encapsulated in a [GNRphenIrCp*OH_2] 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

Planned Milestones and Status: FY17 and FY18

Project Milestone	Type	Task Completion Date				Progress Notes
		Original Planned	Revised Planned	Actual	% Complete	
Use QMC, DFT, and force fields to compute H_2 binding and select appropriate levels of theory for MOFs. Revised milestone: Compute H_2 binding curves with different computational methods for model MOFs to establish protocol for accurate physisorption calculations	PM	12/31/17	3/31/18		70%	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.
Sensitivity analysis of local binding and second-sphere effects	PM	3/31/17		9/30/17	100%	Completed by Maciek Haranczyk (LBNL) for open metal sites in MOFs. Results to appear in sorbent perspective
Rank improvement strategies for sorbents. Decision criterion: select 2 with greatest potential for increasing $\Delta H°$	GNG	3/31/17		3/31/17	100%	Strategy and results reported at AMR. Manuscript for submission to *En. Env. Sci.* in progress
Modify LEIS instrument to enable laser-induced thermal desorption	PM	6/30/17		6/30/17	100%	Demonstrated feasibility of ion beam-based desorption technique
Evaluate additive/composite strategies for improving effective ΔE	PM	9/30/17	9/30/18		75%	Evaluation of multiple strategies in progress

PM=progress measures; M=SMART milestone; GNG=Go/No-go.

Planned Milestones and Status: FY17 and FY18

Prototype hydride surface and interface chemistry kinetic models	M	9/30/17		9/30/17	100%	
Amorphous phases and defects model formalism	PM	12/31/17		12/31/17	100%	
Sensitivity analysis of morphology and microstructure	PM	3/31/18		3/31/18	100%	Completed analysis, reported in LLNL AMR slides
Rank improvement strategies for hydrides. Decision criterion: select 2 with greatest potential for reducing effective ΔH	GNG	3/31/18		3/31/18	50%	Nanoscaling and Dopants addressed experimentally
Parameterize integrated kinetic model for representative B-N-Al-hydrides	PM	6/30/18			75%	Thermodynamic parameters completed. Some kinetic parameters have been calculated for Na-Al-H and Mg-B-H
Compute sorbent isotherms from QMC data using CoRE database of MOFs Milestone delayed until Phase 2 due to lack of personnel with requisite expertise	PM	9/30/18			0%	Not started
Public release of codes, databases, synthetic protocols, characterization methodologies optimized for storage materials Revised language: Public release of databases, synthetic protocols, characterization methodologies optimized for storage materials	M	9/30/18			0%	Not started. Release of codes is a time-consuming process that will be difficult to complete for codes that as of the date of this report are not ready.

PM=progress measures; M=SMART milestone; GNG=Go/No-go.

HyMARC Collaboration and Funding Partners

Sandia National Laboratories

Lawrence Livermore National Laboratory

HyMARC

Hydrogen Materials Advanced Research Consortium

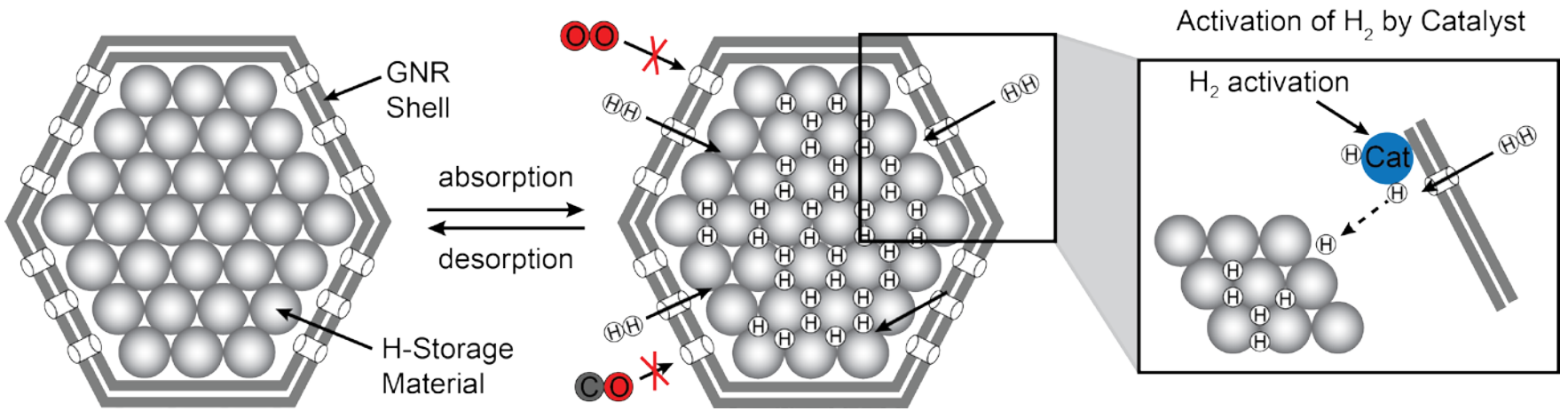
Enabling **twice the energy density** for onboard H_2 storage

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

BERKELEY LAB
Lawrence Berkeley National Laboratory

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_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_2 dissociation/association catalysts at the GNR nanoparticle interface?

Remaining challenges and future plans for soft x-ray spectroscopies @ ALS (Guo)

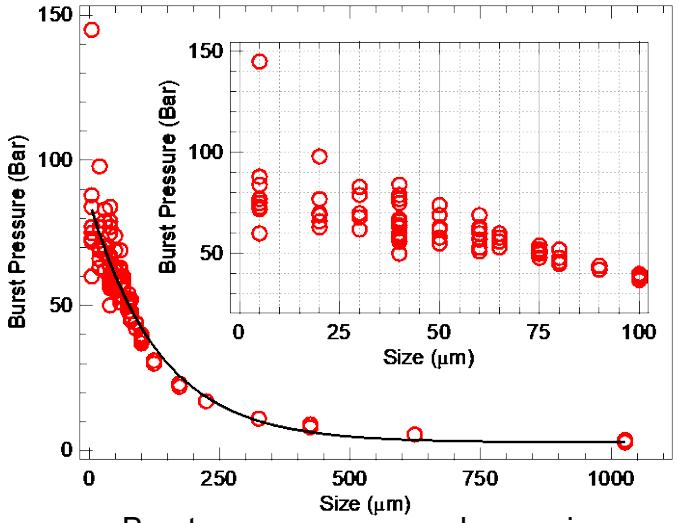
Performing in-situ soft x-ray spectroscopies achieving realistic hydrogen storage are extremely challenging (i.e. UHV requirement)

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)



Burst pressure vs. membrane size

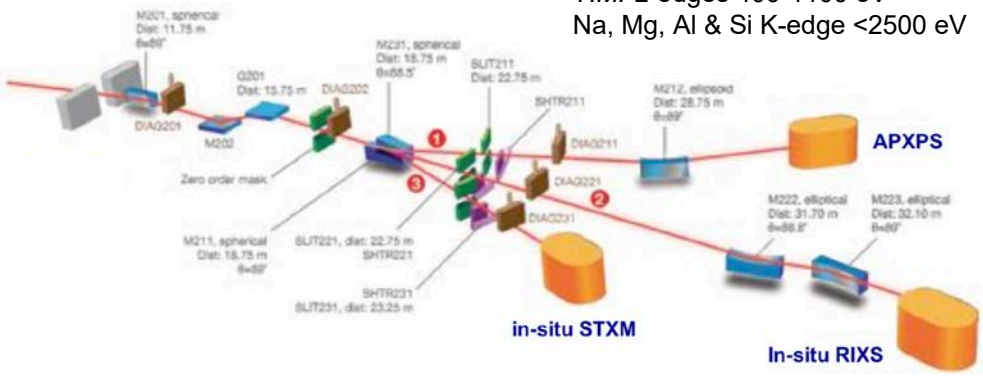
In-situ XAS & RIXS Beamlines

- 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

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



AMBER Endstation