HyMARC: LLNL Technical Activities

2019 DOE Hydrogen Annual Merit Review

May 1, 2019

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HyMARC
Hydrogen Materials Advanced Research Consortium

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

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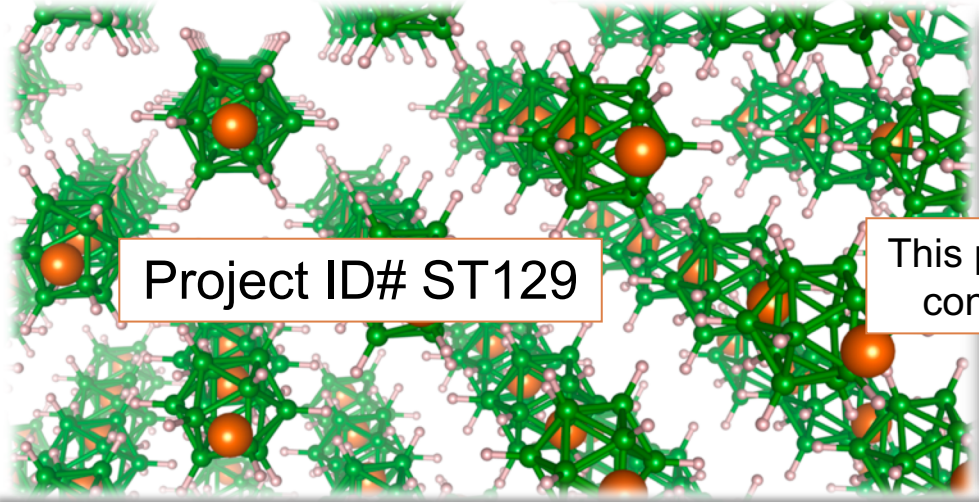
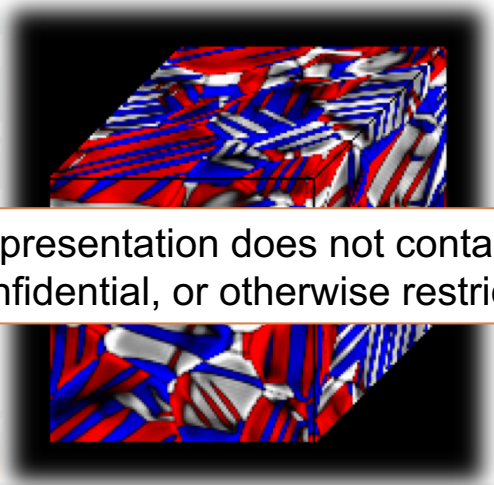


Project ID# ST129



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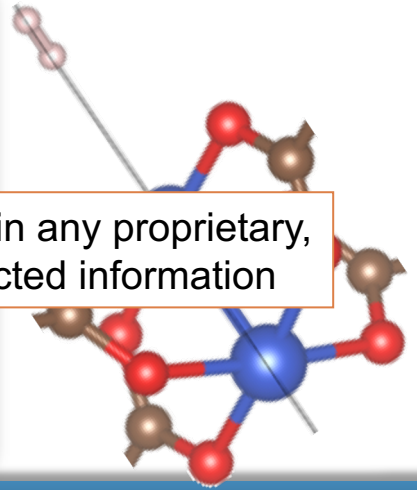

LLNL-PRES-768046

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Lawrence Livermore National Laboratory

Overview

Timeline

Phase II start date: 10/1/2018

Phase II end date: 9/30/2022

Barriers addressed

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

Budget

FY18 Phase I funds: $800K

FY18 Phase II funds: $750K

FY19 funds through 3/31/19: $450K

Partners

Sandia (lead)

NREL (lead)

PNNL

LBNL

NIST

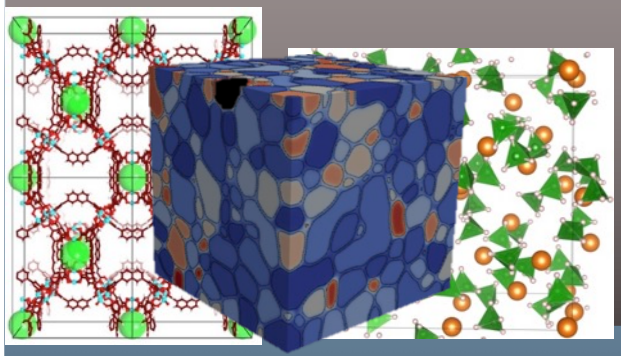
SLAC

ORNL

Relevance

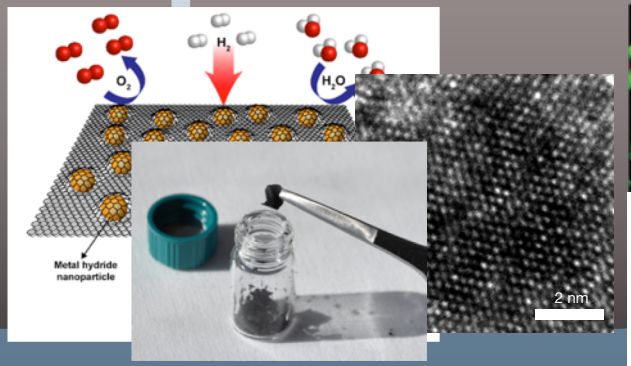
HyMARC improves understanding of underlying thermodynamic and kinetic limitations and explores new concepts to accelerate development of storage materials and carriers

Theory, simulation, data



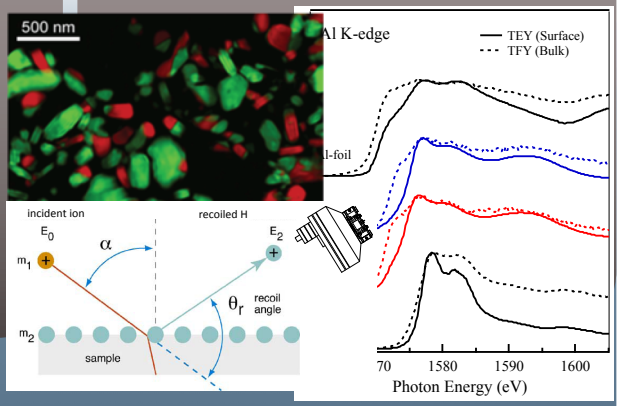
- High-accuracy physisorption
- Phase diagram prediction
- Catalyst pathway and microkinetic models
- *Ab initio* molecular dynamics and spectroscopy modeling for chemistry
- Non-equilibrium mass transport
- Nanoconfinement and interface effects
- Phase-field models for phase transformation kinetics
- Semiempirical kinetic analysis
- Community software & databases

Controlled synthesis



- Functionalized carbon and porous nano-confining media

In situ characterization

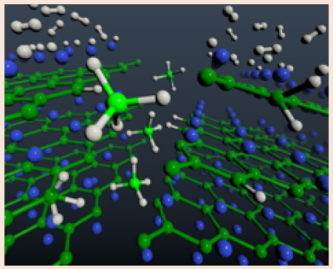


- Soft X-ray absorption & emission spectroscopy
- X-ray spectromicroscopy

Relevance: HyMARC modeling and simulation strategy

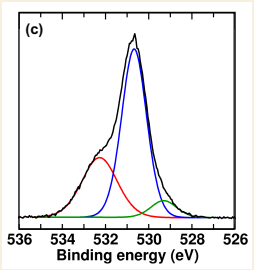
Realistic multiscale modeling and theory-experiment integration aid materials understanding and design

Assess



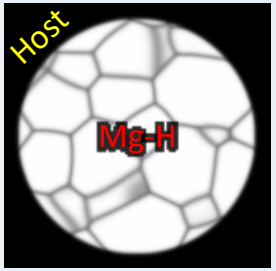
Isolate limiting factors in known materials

Interpret



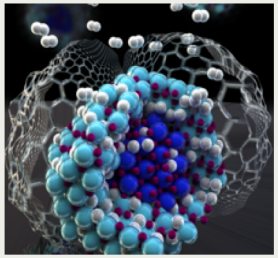
Aid experimental interpretation

Model



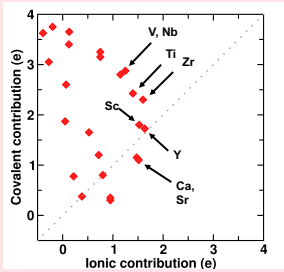
Develop and train models on surrogate materials

Understand



Investigate origins of demonstrated improvement strategies

Design



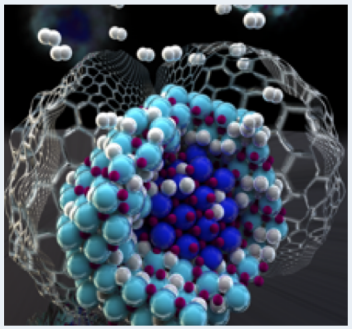
Define theoretical ranges of improvement and design parameters

Approach: Realistic modeling informs improvement strategies

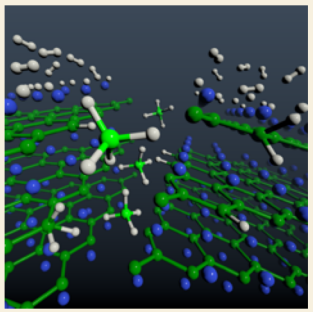
Phase II Tasks

Tuning thermodynamics

- Nanoscaling
- Amorphization
- Mixing
- Confinement



- 2A: Comprehensive phase diagrams for hydride materials
- 2B: Interrogating complex solid interfaces and surfaces
- 2D: Nanoscaling to improve thermodynamics and kinetics
- 3C: Eutectic systems as hydrogen carriers



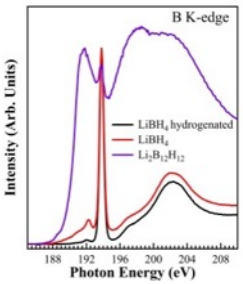
Tuning kinetics

- Catalytic additives
- Nucleation & reaction pathways
- Microstructure
- Host chemical interactions
- Electrocatalysis of H_2 carriers

- 2B: Interrogating complex solid interfaces and surfaces
- 2C: Activating B-B & B-H bonds
- 2D: Nanoscaling to improve thermodynamics and kinetics
- 2E: Microstructural impacts on metal hydride reactions
- 3H: Catalyst stability

Approach: Simulation of hydrides at multiple scales

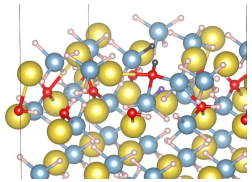
Atomic/molecular (0 – 1 nm)

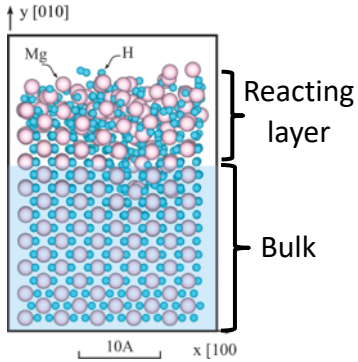


Computational Spectroscopy

Hydrogen physisorption

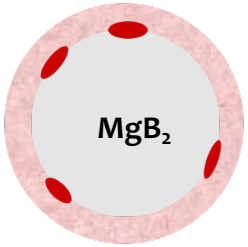
Molecular/micro (0.5 – 2 nm)

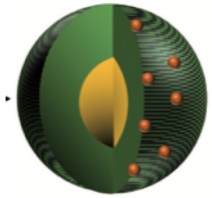




Surface/interface chemistry

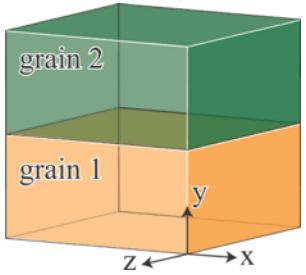
Mesoscale (2 - 100 nm)





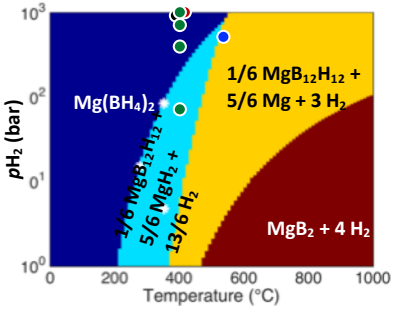
Nucleation kinetics
Phase microstructures

Grains (≤ 10 µm)



Grain boundaries
Particle size effects
Stress/strain

Macroscale/Bulk



Thermodynamics
Mixing

Density functional theory & ab initio molecular dynamics	*Classical molecular dynamics & microkinetic modeling*	*Phase-field modeling & microelasticity*	*Ab initio thermodynamics*

10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2}

Length (m)

Progress towards FY19 milestones with key LLNL activities

FY19Q2: Generate DFT training set for B_xH_y-cation interactions to formulate pair potentials (70%)

- *Formulated basic molecular training set and initiated three complementary strategies for pair potentials*

FY19Q4: Perform molecular dynamics of surfaces of complex hydrides (20%)

- *Generated static surface models to be used as inputs for dynamics simulations*

FY19Q3: Develop computational approach for screening additives to activate B-B bonds in MgB_2 (80%)

- *Preparing publication on B-B bond interactions in MgB_2 with metal additives; currently validating with experiments*

FY19Q4: Determine theoretical limits of confinement-induced enthalpy and entropy changes (50%)

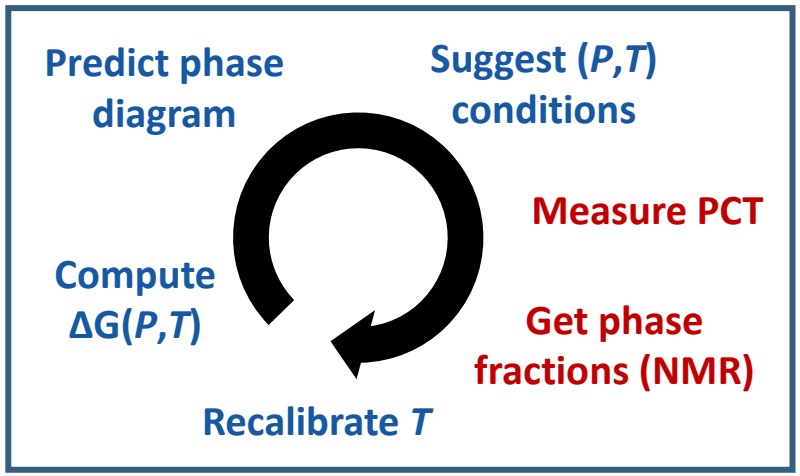
- *Surface energies computed; entropy will follow upon completion of surface dynamics*

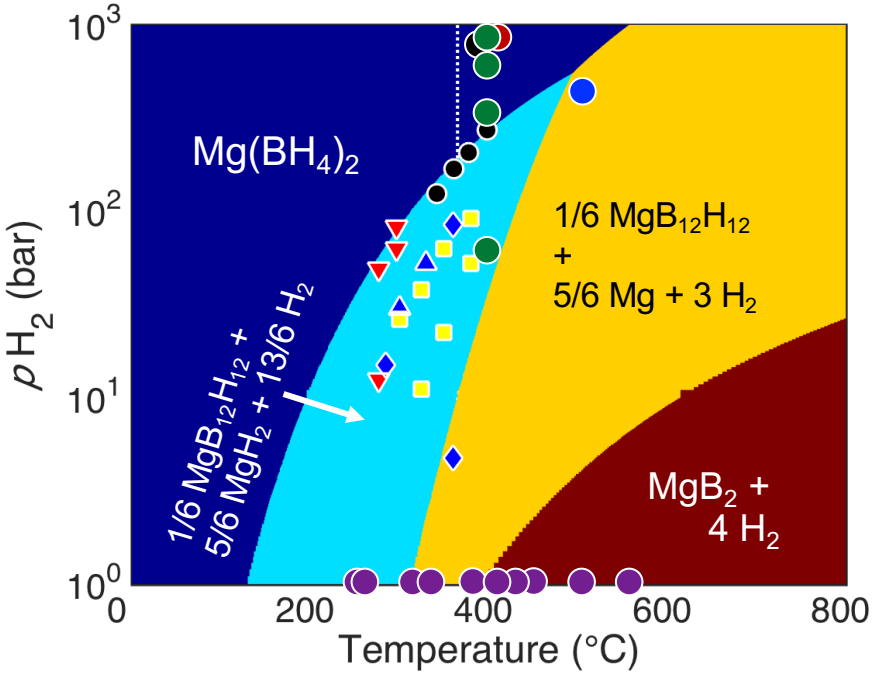
FY19Q4: Predict possible microstructure morphologies based on nucleation model and compare with STXM to elucidate kinetic pathways (70%)

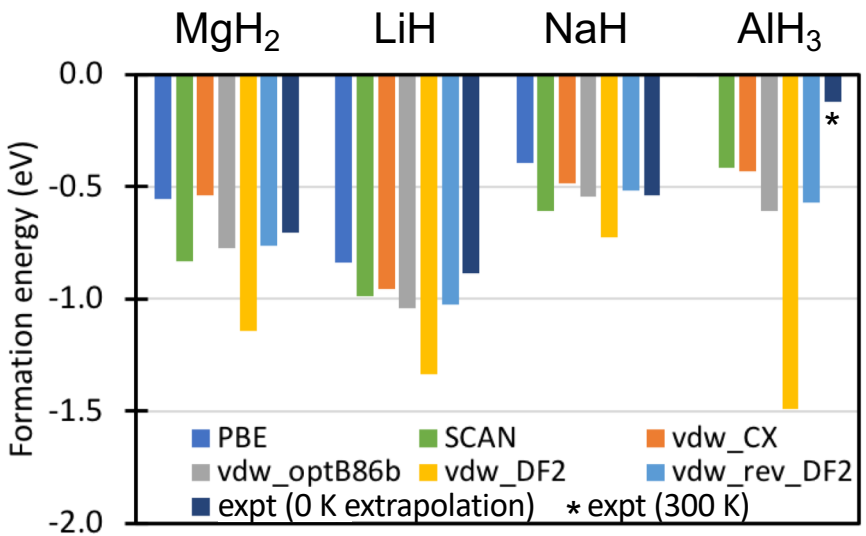
- *Determined three unique microstructures based on barriers in multi-stage nulceation*

Bulk phase diagram prediction and validation

We continue to refine phase diagrams through experiment-theory feedback cycle





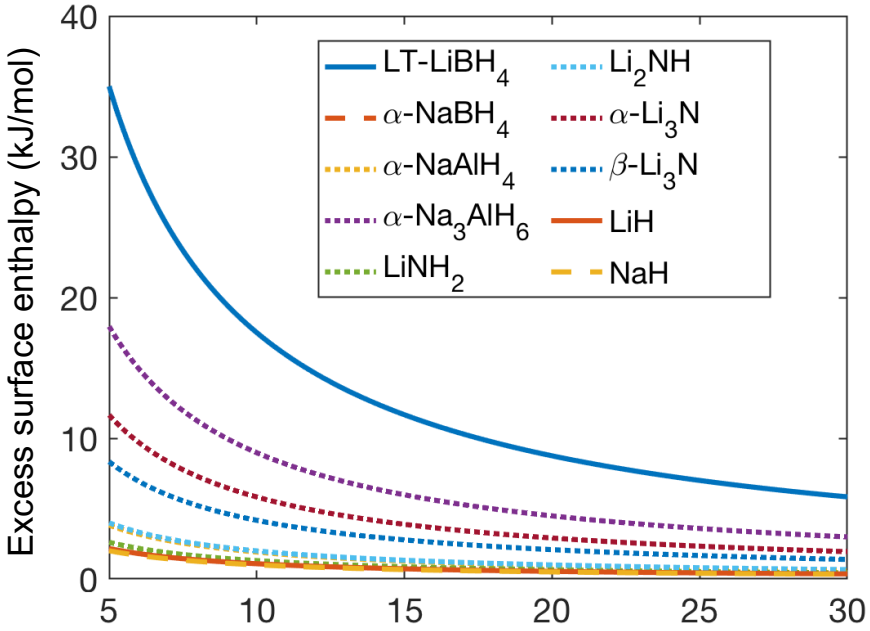


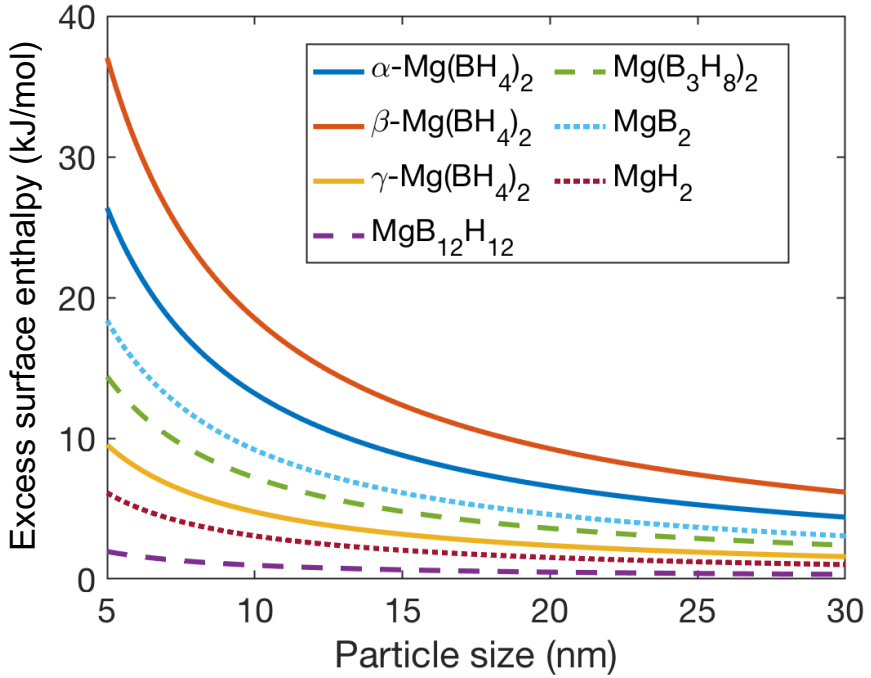
Entropy is predicted to within experimental accuracy using our latest approach, but we are pursuing higher accuracy for enthalpy

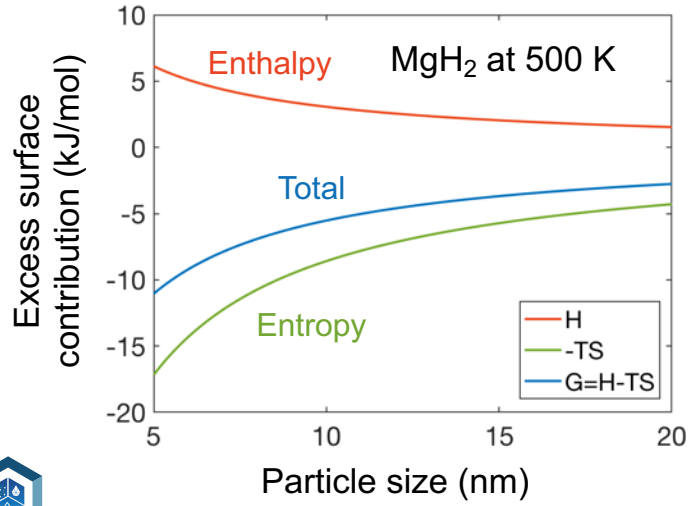
- Data-driven corrections
- New density functionals

Assessing effects of nanoscaling on thermodynamics

We are using surface enthalpy and entropy to predict tunability limits of nanoscaling



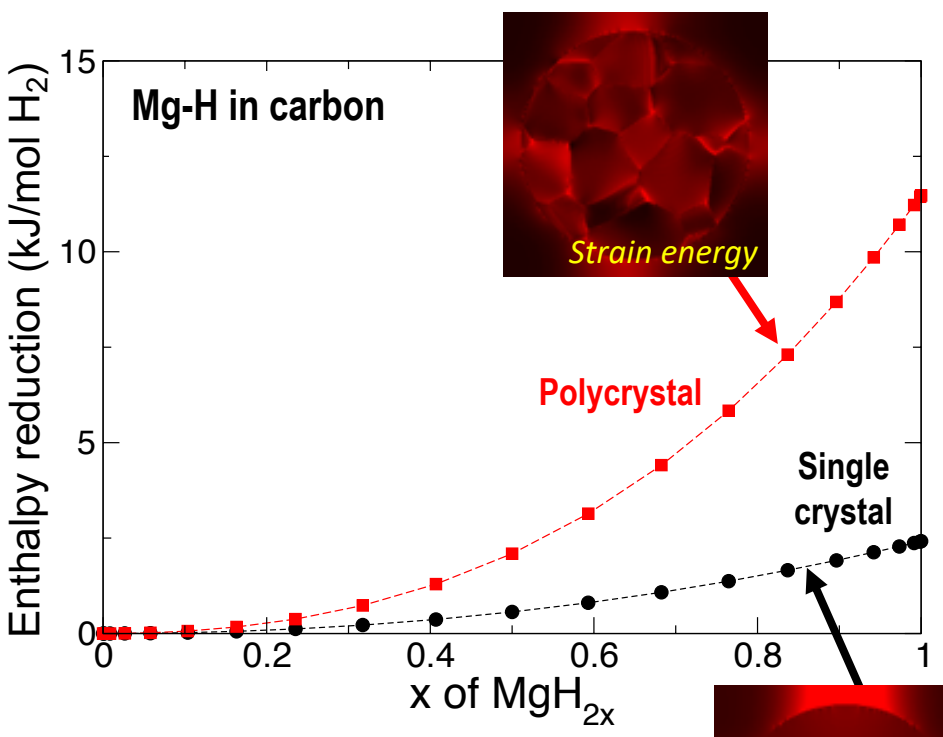




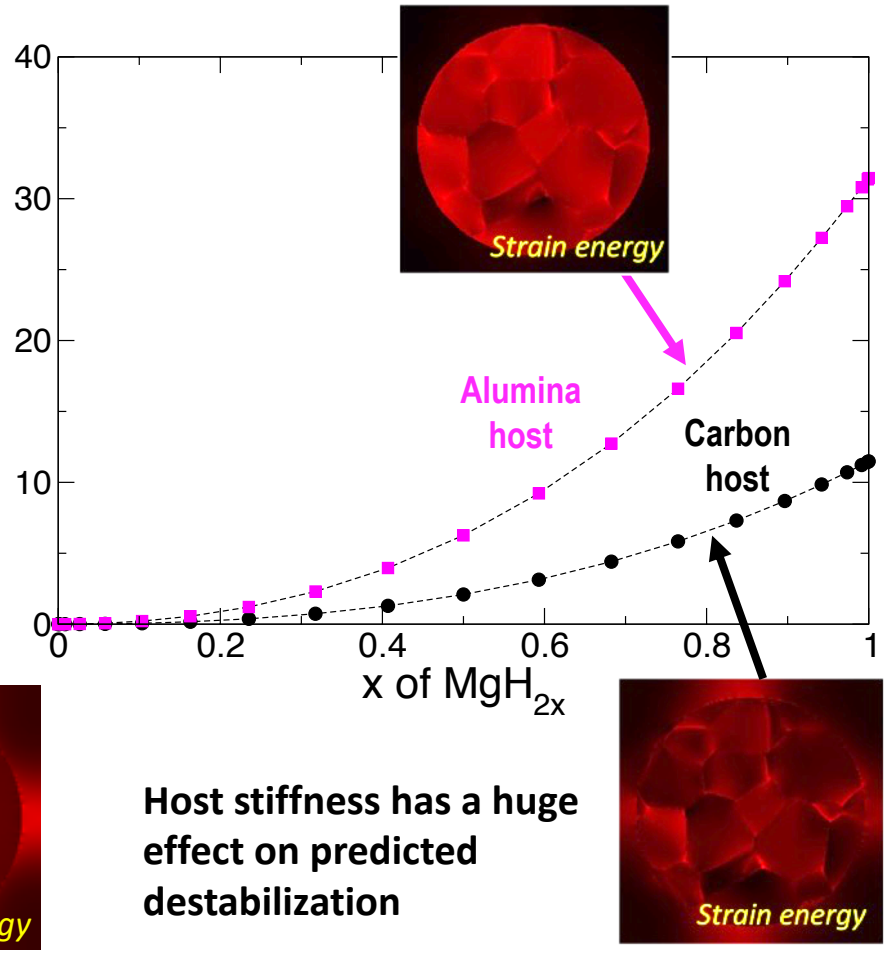
Excess surface entropy explains enthalpy-entropy compensation effect in nanoscale metal hydrides

Confinement stress: Promising strategy for destabilizing hydrides

We enhanced our confinement stress model to account for more realistic microstructures and variable host elasticity, which show large effects on thermodynamics and kinetics



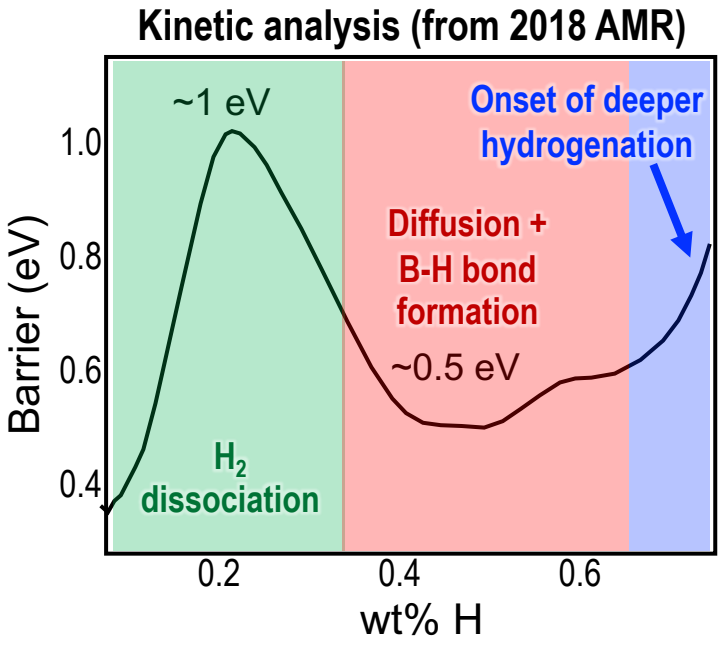
Polycrystalline systems exhibit much higher local stresses, which can enhance local kinetics

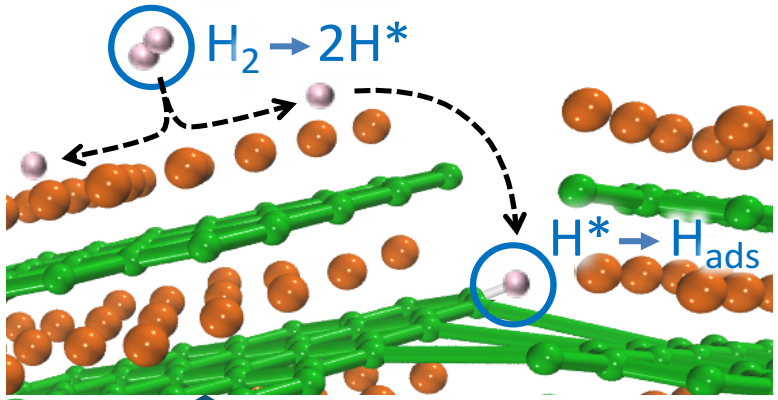


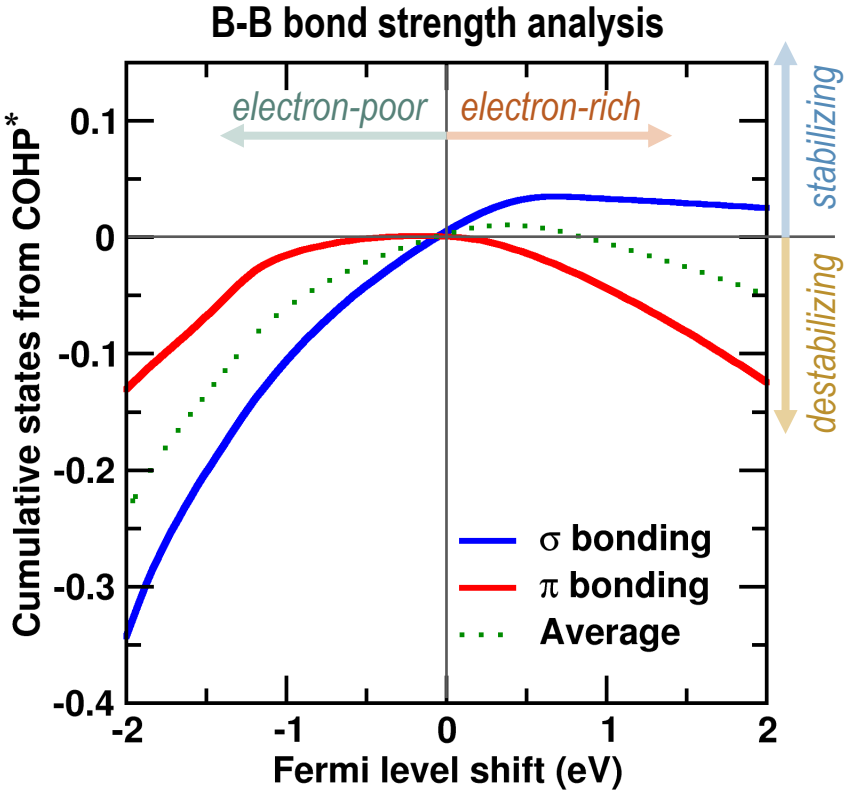
Host stiffness has a huge effect on predicted destabilization

Understanding and accelerating MgB_2 decomposition

Hydrogenation beyond ~0.8 wt.% H is not limited by B-H bond formation or H_2 dissociation (confirmed by H-D isotope exchange); instead, likely limitation is from B-B bond cleavage







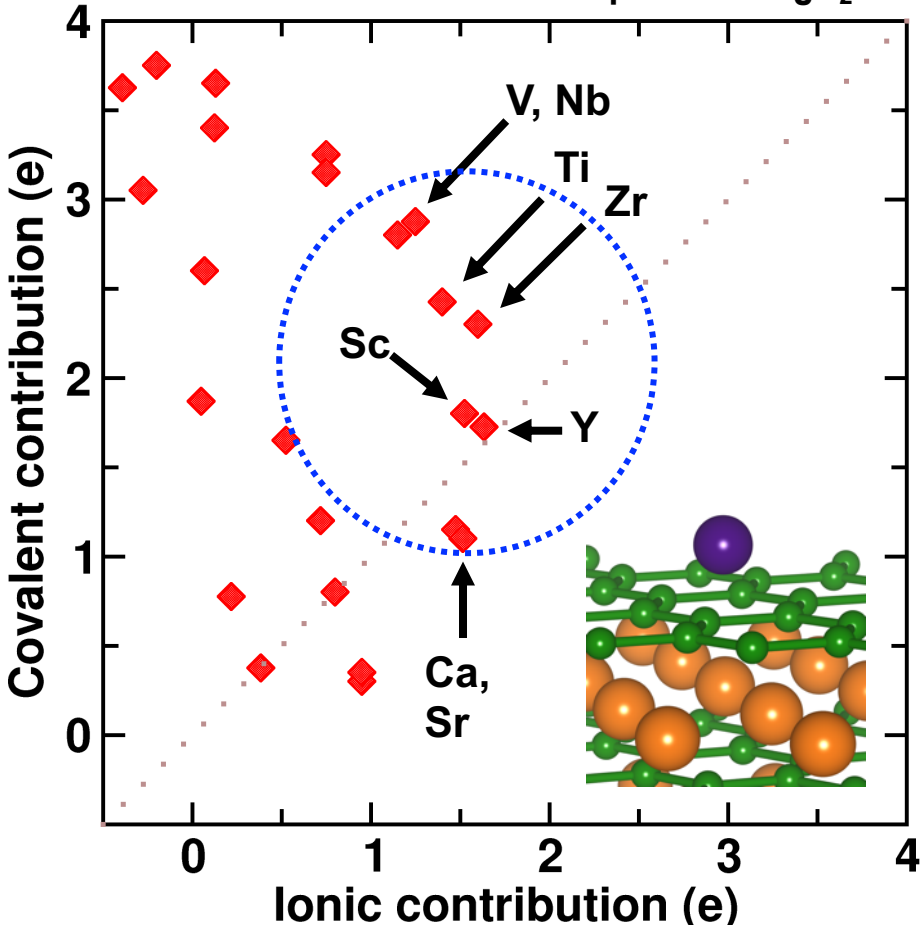
B-B bonds are weakened by charge donation/ depletion and/or changes to σ-bonding states.

Similar effect can be achieved by extracting Mg^{2+}, which may explain functionality of solvents.

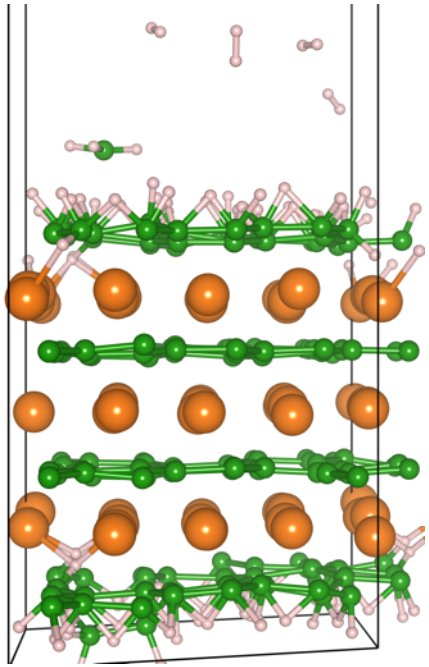
Screening metal dopants with mixed ionic-covalent character

Metal dopants for accelerated MgB_2 decomposition should mix charge donation (ionic bonding) with covalency to alter σ-bonding states

Bonding contributions for alkali, alkaline earth, & 3d/4d transition metal dopants on MgB_2



Changes in B-B XAS bond signature for MgB_2 ball-milled with dopants provide validation (early results on Ti vs. Li agree with predictions)

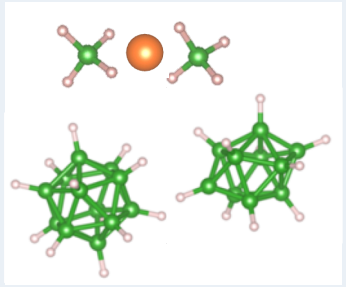


Effect on hydrogenation is being investigated via Sieverts testing and ab initio MD

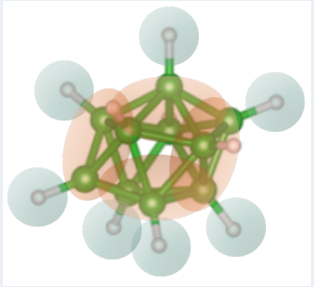
Complex hydrides: *ab initio* calculations inform scalable methods

Classical B_xH_y potentials

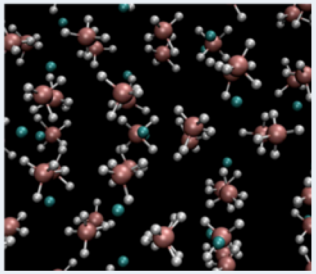
Rigid pair potentials (w/Sandia)



SAPT potentials (w/Georgia Tech)



Machine learning from dynamics trajectories (w/Tennessee State)

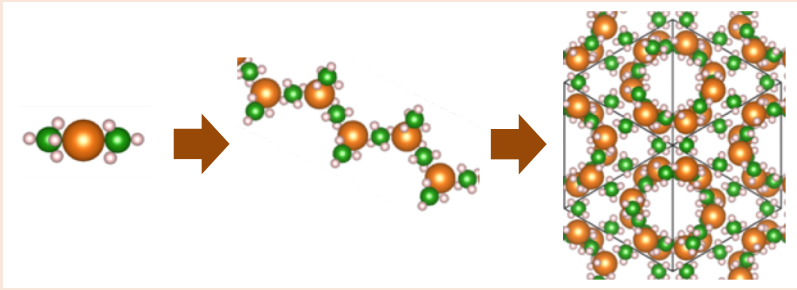


Will be used to compute energetics of:

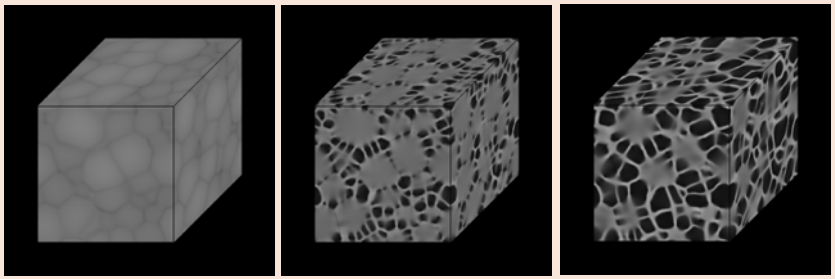
- *Complex interfaces*
- *Mixtures/alloys*
- *Amorphism*
- *Polymorphism*

Parameterized mesoscale simulations

Nucleation kinetics



Interfacial energies & solid mechanics

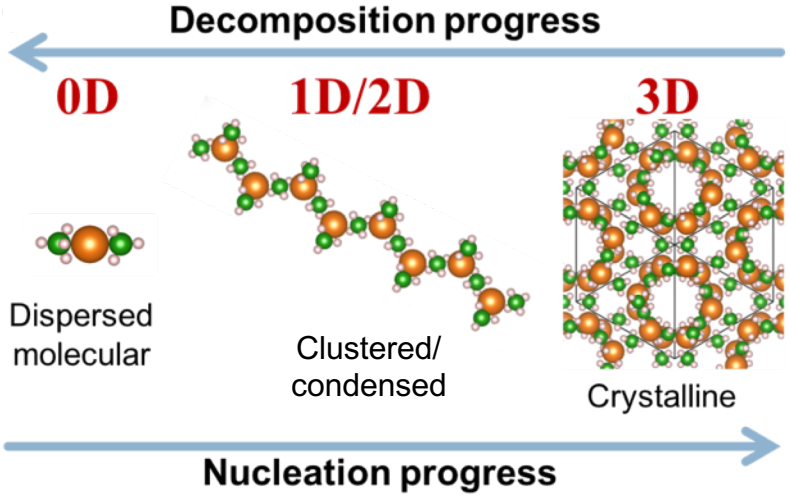


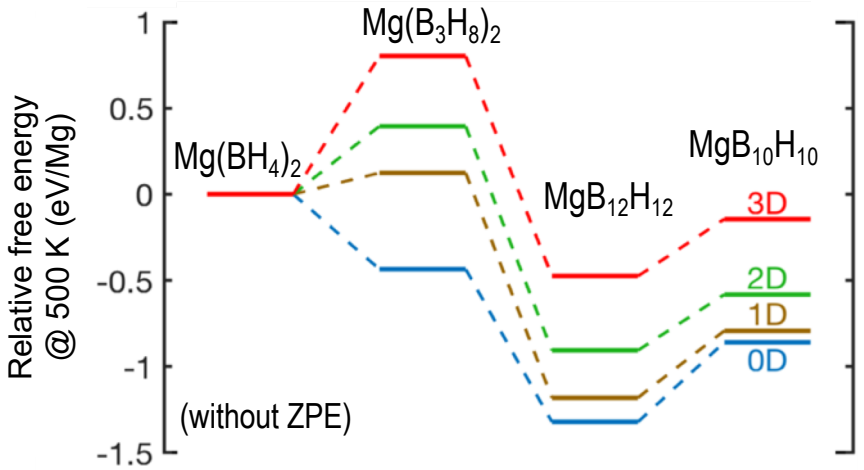
Will be used to compute kinetics of:

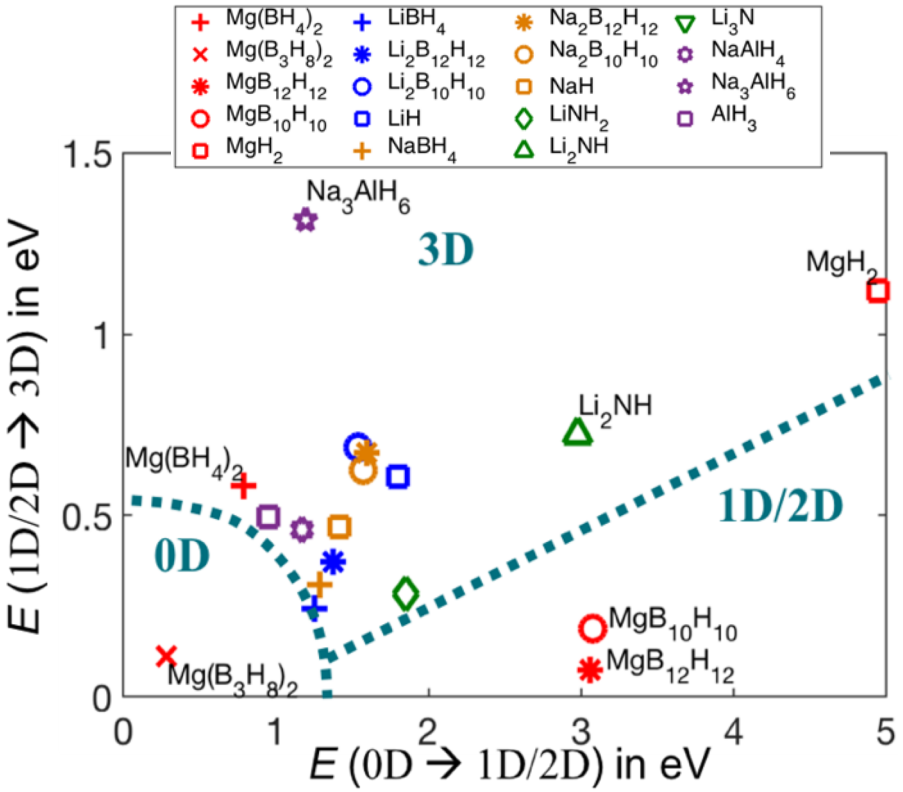
- *Isotherm uptake*
- *Microstructure evolution*
- *Mass transport*

Clustering and nucleation of intermediates

Comparisons of energetics at different "dimensionalities" from molecular to crystalline provide insights into nucleation and how reaction pathways can be tuned by morphology







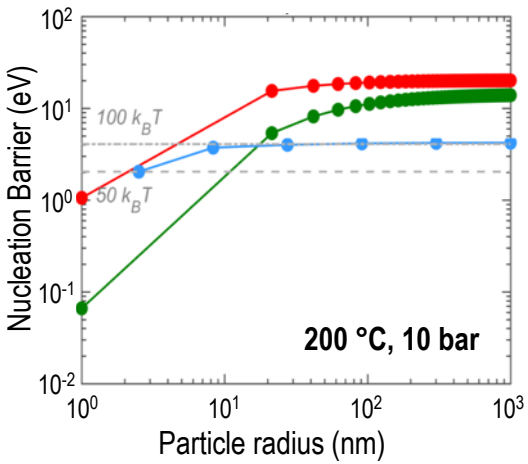
Driving force for crystallization relates to chance of forming solid solution with faster phase kinetics

Explains observations of metastable intermediates (e.g., $Mg(B_3H_8)_2$) that do not appear as crystalline

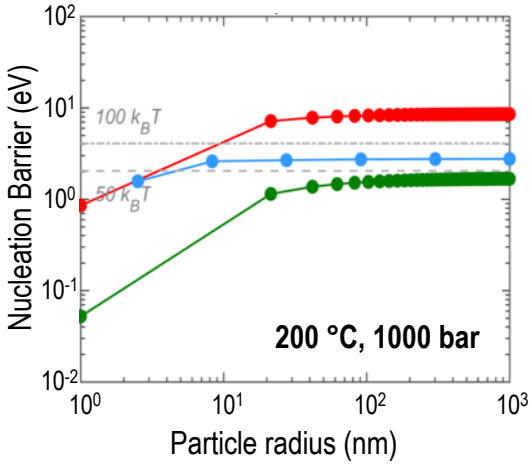
Nucleation kinetics models reveal solid phase pathways

Kinetics favor two-step condensation-crystallization mechanism of $Mg(BH_4)_2$ formation with pressure-dependent rate limitation

Low H_2 pressure: Chemical kinetics limit rate



High H_2 pressure: Crystallization limits rate

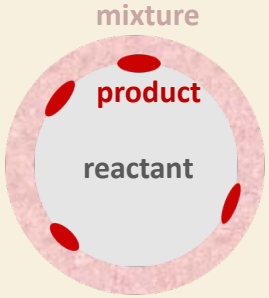


Identified three different microstructures generated by different energy landscapes

Unstable intermediates

High barrier for decomposing intermediates

High barrier for forming intermediates

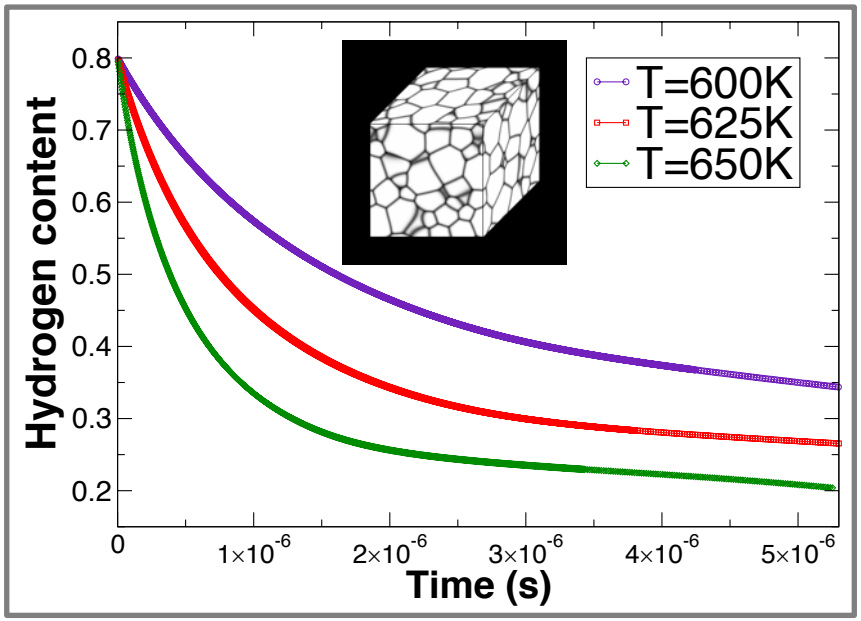


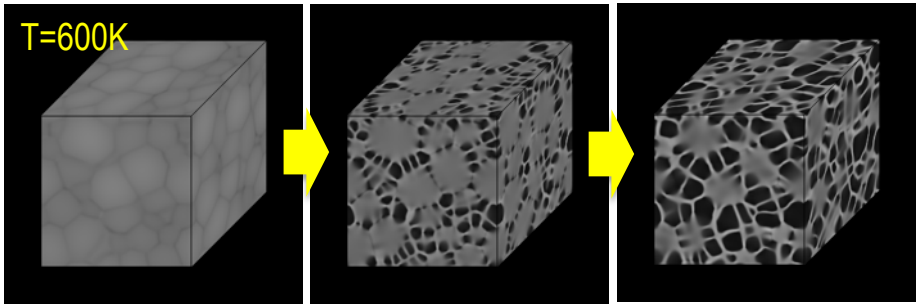
Comparisons with STXM on Li-N-H and Mg-B-H are underway

DRINK model progress: PdH_x dehydrogenation kinetics

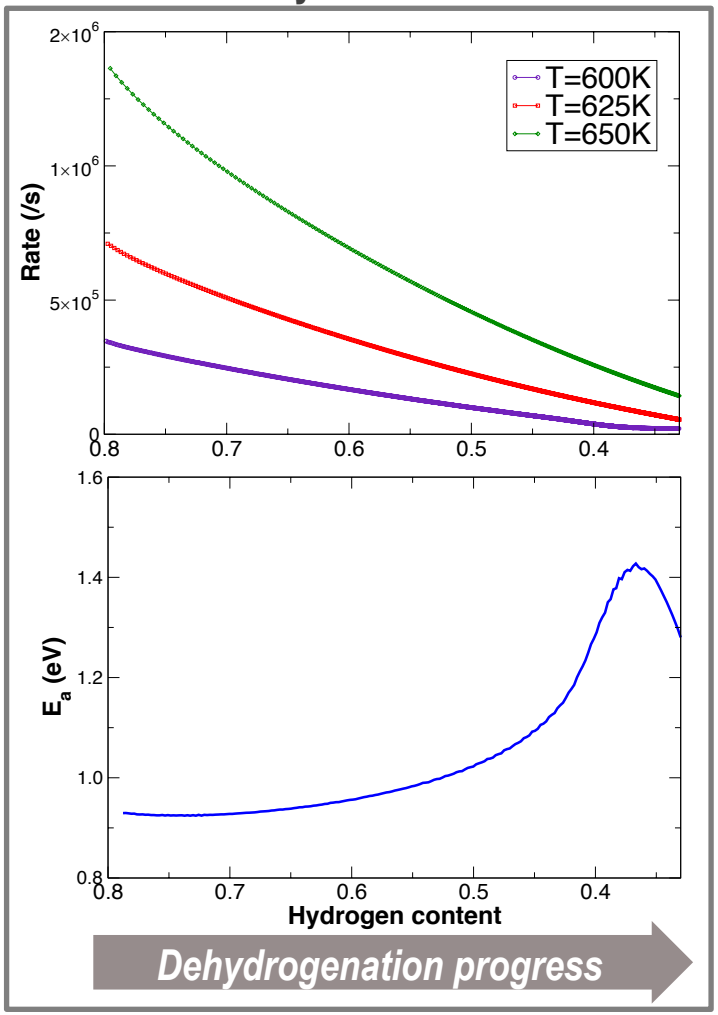
Diffuse Reactive Interface Nonlinear Kinetics model integrates chemistry, diffusion, stress, and phase transformations to simulate full reaction and identify rate-limiting factors

Simulated dehydrogenation



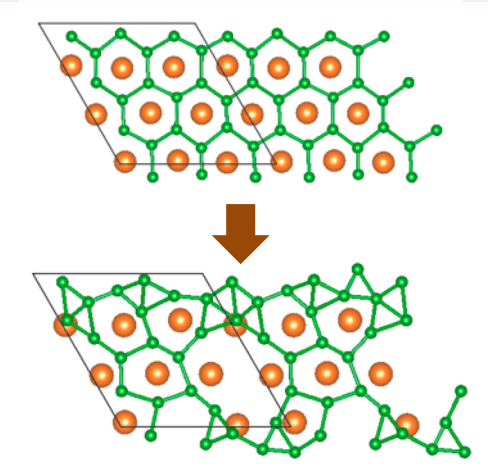


Kinetic analysis of simulations



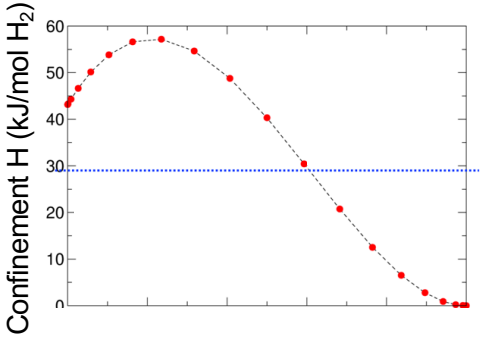
Highlights of interactions with seedlings

Severa, U. Hawaii (MgB_2/ethers)



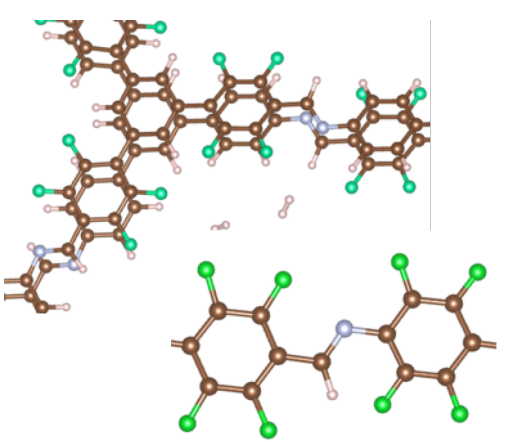
- Regular monthly meetings
- Discovered mechanism of MgB_2 decomposition
- Investigated anthracene, THF, and inorganic additives

Christensen, NREL ($Mg(BH_4)_2$ @ ALD oxides)



- Hosted in-person meeting 11/18
- Estimated stiffness-dependent confinement and showed faster rates are from oxide reactions
- Follow-up simulations planned

Johnson, NREL (COFs)



- Regular monthly meetings
- Computed functionality-dependent H_2 binding and structural stability in COFs

Vajo, LiOx/Caltech (Electrolyte + hydrides)

- Phase II kickoff web meeting 1/2019
- Possible origins of solvent effects on MgB_2 decomposition
- Planned simulations of MgB_2 with iodide salts

Collaborations

HyMARC collaborations

- *Multi-lab working group focus areas on Mg-B-H system and nanoconfined hydrides*
- *Extensive collaborations on all topics (see lab logos on slides)*

U.S. collaborations

Michigan State (Prof. Hui-Chia Yu)
- *Energy landscape interpolation for phase-field model development*

Georgia Tech (Prof. Jesse McDaniel)
- *Symmetry-adapted perturbation theory (SAPT) potential development for $B_xH_y^{n-}$*

Tennessee State (Prof. Lizhi Ouyang)
- *Machine learning for structure prediction and potential development for Li/Na/MgB_xH_y compounds*

U. South Carolina (Prof. Morgan Stefik)
- *Confinement stress effects on hydride thermodynamics*
- *New NSF partnership with HyMARC*

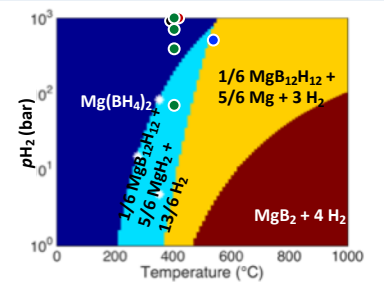
Foreign collaborations

KAIST, Korea (Profs. Eun Seon Cho, Seung Min Han, and Bong Jae Lee)
- *Microstrain and thermal transport in confined metal hydrides*
- *Multi-institutional partnership launched in September 2018*
- *Held workshop in October 2018 to draft CRADA*

AIST, Japan (Minoru Otani)
- *Hybrid quantum-classical simulations of catalytic interfaces for hydrogen carriers*

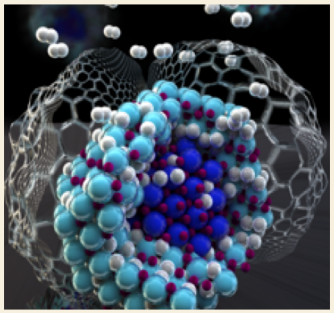
Helmholtz Zentrum Geesthacht (Martin Dornheim, Anna-Lisa Chaudhary)
- *Mixed metal hydride reactions and phase evolution*
- *Held workshop in December 2018 to identify research partnerships*

Proposed future work



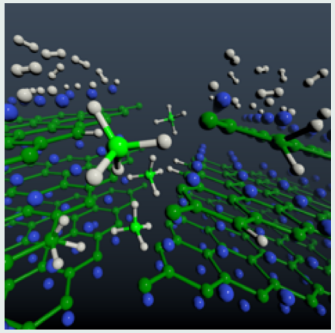
Phase diagram prediction/validation

- Establish **best practices** for DFT enthalpy predictions across multiple hydrides
- Complete **surface entropy** calculations for computation and validation of **size-dependent phase diagrams**



Tuning thermodynamics

- Apply new potentials to predict free energies of Li/Na/MgB_xH_y **eutectic mixtures**
- Estimate and validate potential of **amorphization** to alter ΔH and ΔS
- Validate size-dependent tunability for key hydrides by deconvoluting contributions of **surfaces and confinement stress**

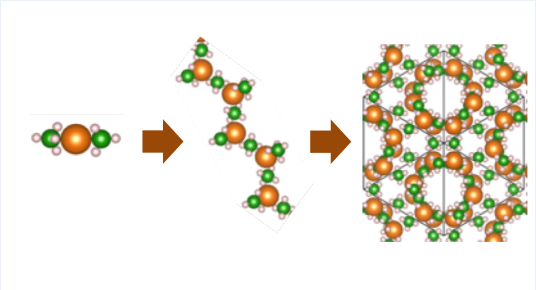


Tuning kinetics

- Extend **additives** study to dehydrogenation and continue model validation alongside direct *ab initio* molecular dynamics simulations
- Compute **Lewis acid/base interactions** with oxide hosts
- Compute **nucleation barriers** for Li-N-H and compare **microstructures** with STXM
- Parameterize **DRINK model** for partial hydrogenation of complex hydride
- Compute reaction landscape and catalyst stability for **formate and formic acid** electrocatalysis (H_2 carriers)

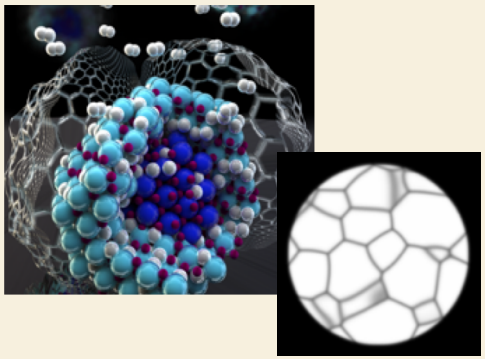
Summary: Moving the bar on metal hydrides

New tools & capabilities



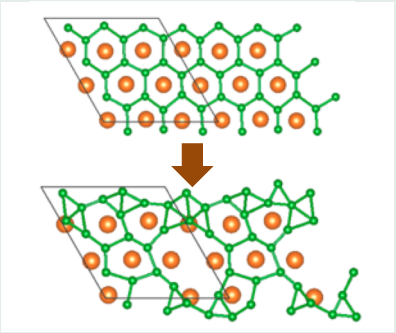
- Clustering and crystallization energies from morphology-dependent thermodynamics
- Advanced nucleation model
- Diffuse Reactive Interface Nonlinear Kinetics (DRINK) model

Materials tunability & design



- Quantified surface influence on nanoscale hydride enthalpy
- Assessed effects of crystallinity and host stiffness on confinement enthalpy
- Screened metal additives for effect on MgB_2 destabilization

New foundational understanding



- Showed origin of enthalpy-entropy compensation for nanoscale hydrides
- Demonstrated charge-reactivity interplay in MgB_2
- Determined link between nucleation pathways and microstructure

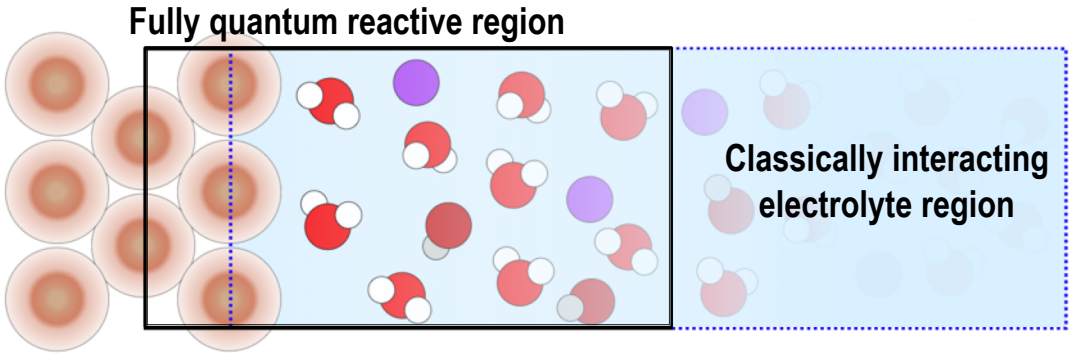
Also authored theory sections in new reviews on nanoscale hydrides and sorbents

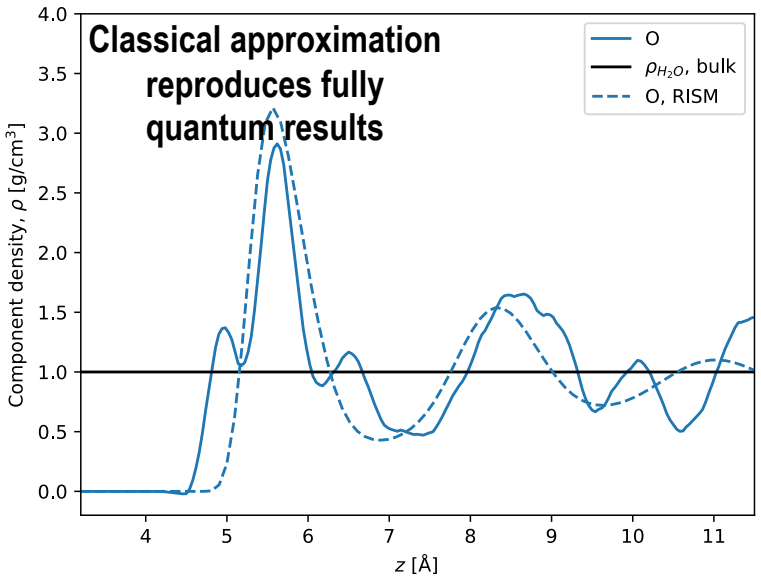
Technical backup slides

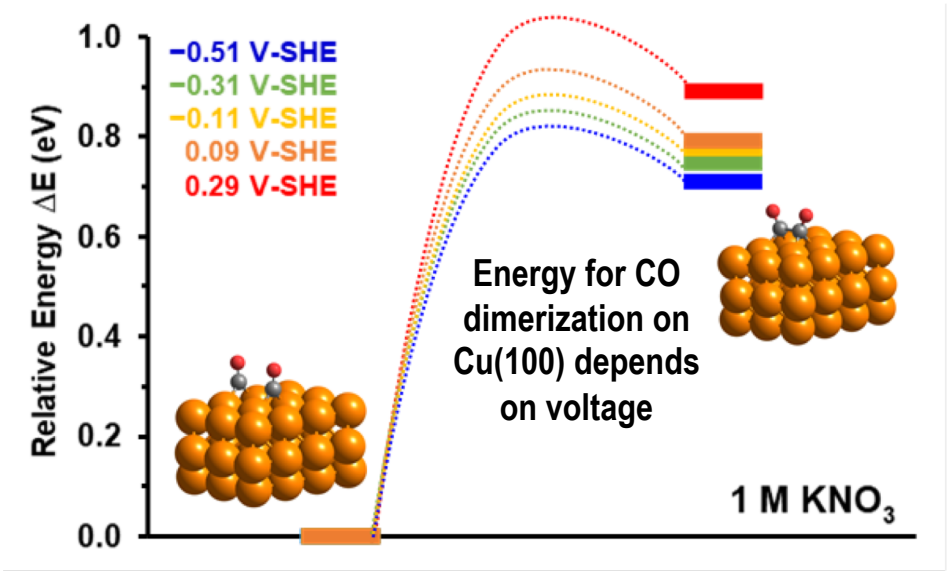
Benchmarking theory for electrocatalysis of H_2 carriers

We are exploring quantum-classical hybrid approaches for computing electrocatalytic overpotentials and voltage/temperature effects on formate and formic acid production

ESM+RISM Method (w/AIST Japan)

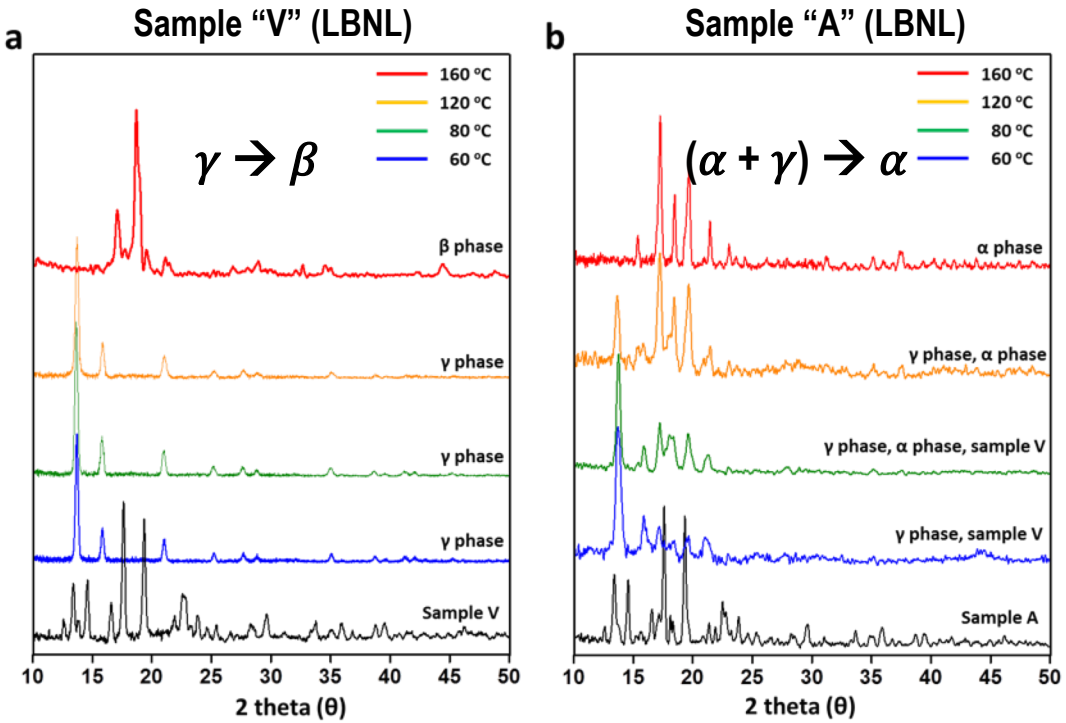


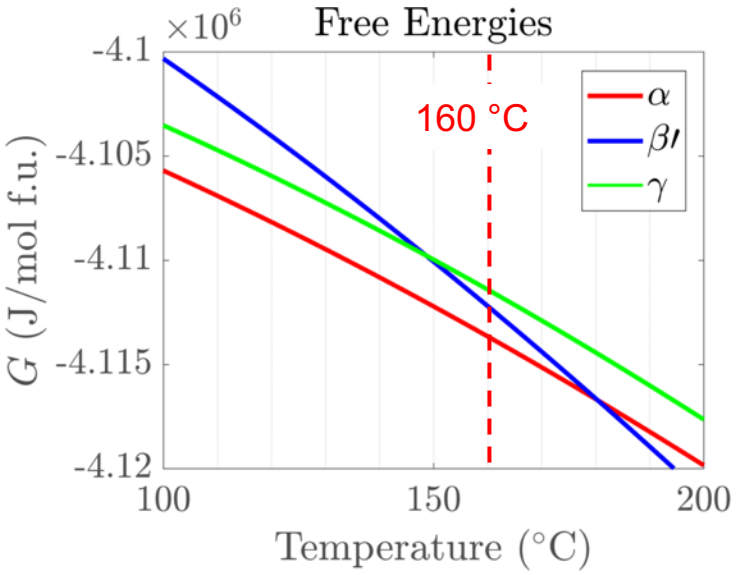




Tuning pathways via nucleation: Polymorphism in $Mg(BH_4)_2$

We are working with LBNL to understand polymorphic phase expression in $Mg(BH_4)_2$ under different synthesis conditions by applying our advanced nucleation model

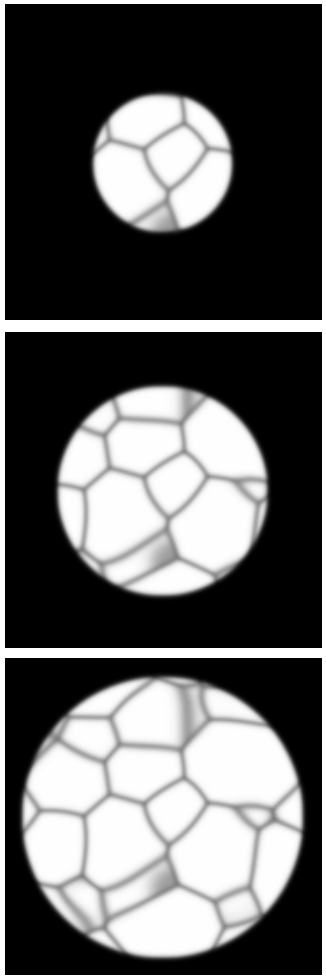


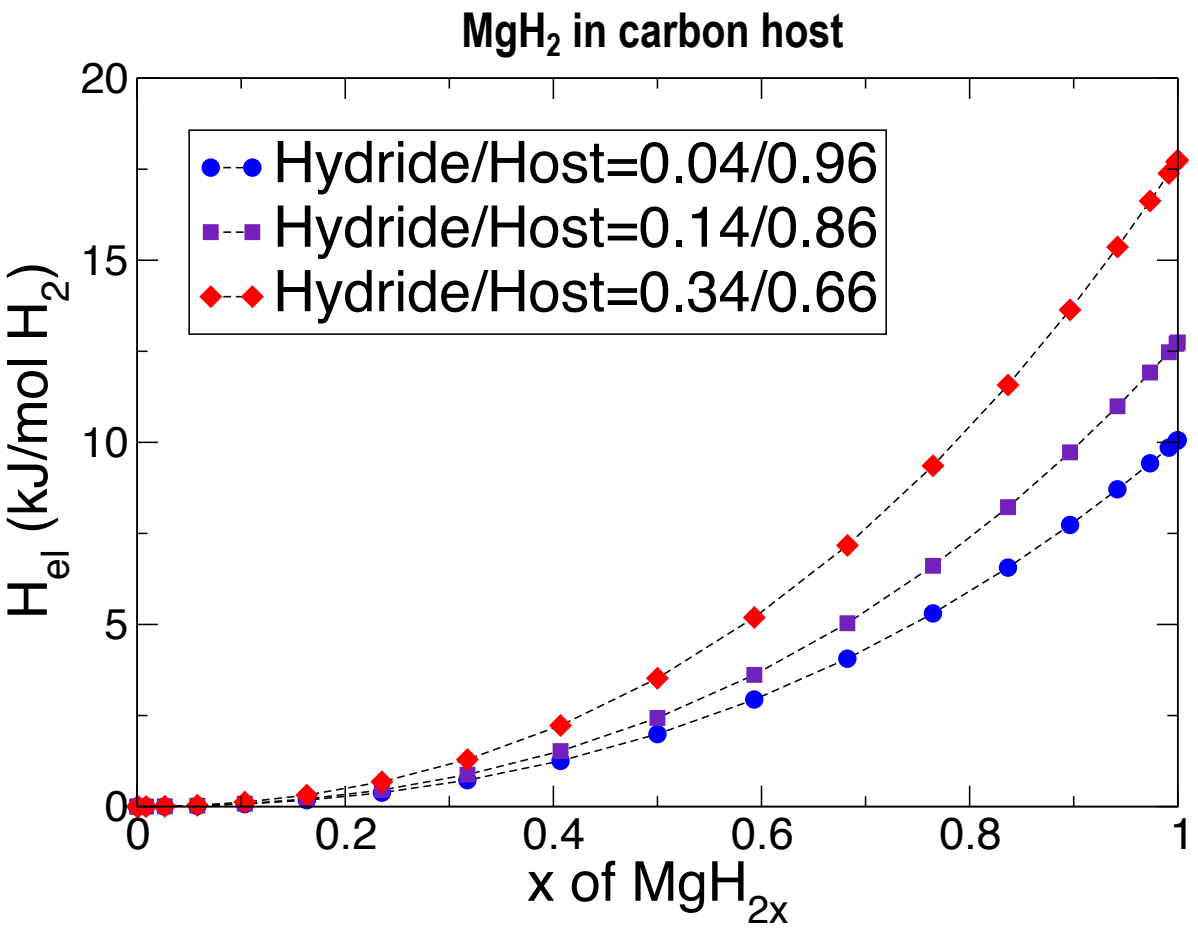


Different nucleation barriers for different polymorphs accounts for observed phase expression (manuscript in preparation)

Confinement stress: Effect of hydride loading

Higher hydride loading in carbon significantly enhances enthalpy destabilization





This same framework can be used to study the effects of powder packing density on hydride confinement stresses

Reviewer-only slides

Challenges/barriers, critical issues, and mitigation strategies

- **Microstructural information is needed for nucleation model validation**

  We have started collecting STXM data, but proper interpretation has been challenging. To this end, we continue to collect standards for unambiguous deconvolution of phases.

- **More realistic structural models of metal additives may be necessary**

  Our current models rely on single-atom adsorbates. However, for the most promising candidates in our screening, we are now starting calculations of substitutionally incorporated metals and full interfaces with metal crystallites to determine whether our conclusions hold.

- **Difficult to isolate and validate confinement stress effect**

  Currently, it is difficult to deconvolute the effects of surface enthalpy from confinement stress for nanoconfined hydrides. The new NSF project by Prof. Stefik (U. South Carolina) will focus on this aspect by tuning scaffolds with varying thicknesses and pore sizes.

- **Difficult to isolate and validate individual kinetic factors**

  We continue to explore advanced experimental methods for isolating kinetic factors. However, our general simulation approach involves using microscopic kinetic predictions to parameterize a full simulation of hydrogen uptake/release isotherms via the DRINK model. Although this approach can only facilitate validation of overall kinetics, we can rely on the model to explore how reaction rates change as individual kinetic factors are adjusted.

Responses to 2018 AMR reviewer comments

- **Comment 1: The team should make every effort to experimentally validate the findings.**
  - Response: This continues to be a priority. The Reviewer specifically mentions spectroscopic validation of B-B bond breaking in the presence of additives, which was performed successfully. We also validated the prediction that H-H dissociation is not rate limiting using isotope exchange experiments. For validating the phase nucleation models, we are comparing predictions with STXM, although the interpretation of the latter remains challenging. In addition, we have an external partnership with KAIST and a new partner NSF project with M. Stefik (U. South Carolina) that are focused on validating the confinement strain models.
- **Comment 2: The weakness of this project is in other length scales compared to atomic scale. The areas of reactive dynamics need more work. The phase-field and grain-boundary phenomena are not at the forefront of this project.**
  - Response: Our feedback for FY17 was that we focused too much on microstructure and not enough on chemistry, so last year we chose to prioritize atomic-scale phenomena within our budget constraints. Nevertheless, the work on larger length scales has continued and is well reflected in this year's slides. We have significantly enhanced the sophistication of our nucleation model (which is now parameterized by atomistic calculations), included a research direction on the effects of polycrystallinity and packing on mechanics and diffusion, and demonstrated the first fully parameterized version of our DRINK reactive interface model that incorporates phase transformation kinetics, diffusion kinetics, and mechanics for direct isortherm simulation.
- **Comment 3: The addition of reactive dynamics is recommended.**
  - Response: We explored complex reactive molecular dynamics methods (e.g., ReaxFF) early in the project but concluded that proper parameterization is extraordinarily difficult, making it very easy to unintentionally bias the results. We instead decided to pursue bond-order potentials for direct hydrogenation of simple and interstitial hydrides (e.g., MgH_2 and PdH_x) and nonreactive classical potentials for complex hydride mixtures and interfaces (rigid-body, SAPT, and machine learning-derived). Our key strategy for bridging scales for reaction kinetics continues to be integration of quantum-accuracy parameters directly into phase-field models. However, as we collect more quantum-accuracy data on transport and phase transformations, we plan to reconsider the addition of reactive MD and DFTB (density functional tight binding) methods, with which our team has some experience.

Responses to 2018 AMR reviewer comments

- **Comment 4: Additional input from the phase-field models needs to be evaluated for the actual strength in predicting physically meaningful insights. Otherwise, much of the phase-field models suffers from unphysical assumptions.**
  - Response: We continue to refine the assumptions that enter the phase-field and nucleation models. Our newest formulation of the nucleation models are parameterized directly from first-principles calculations. In addition, we have now fully parameterized the DRINK model, which is based on the phase-field formalism, for a real system (PdH_x). Finally, in our newest mesoscale confinement models, we have now included complex microstructures and a correctly parameterized elastic response of the confining host, thereby significantly improving the realism of our model.

Publications

1. T.W. Heo and B.C. Wood, “On thermodynamic and kinetic mechanisms for stabilizing surface solid solutions,” in review (2019).
2. L.F. Wan, E.S. Cho, T. Marangoni, P.T. Shea, S. Kang, C. Rogers, E.W. Zaia, R.R. Cloke, B.C. Wood, F.R. Fisher, J.J. Urban, and D. Prendergast, “Edge-functionalized graphene nanoribbon encapsulation to enhance stability and control kinetics of hydrogen storage materials,” in review (2019).
3. S. Kang, T.W. Heo, M.D. Allendorf, and B.C. Wood, “Morphology-dependent stability of complex metal hydrides and their intermediates using first-principles calculations,” *ChemPhysChem*, accepted for publication (2019).
4. X.W. Zhou, S. Kang, T.W. Heo, B.C. Wood, V. Stavila, and M.D. Allendorf, “An analytical bond order potential for Mg-H systems,” *ChemPhysChem*, in press (2019). DOI:10.1002/cphc.201800991
5. J.L. White, A.J.E. Rowberg, L.F. Wan, S. Kang, T. Ogitsu, R.D. Kolasinski, J.A. Whaley, A.A. Baker, J.R.I. Lee, Y.-S. Liu, L. Trotochaud, J. Guo, V. Stavila, D. Prendergast, H. Bluhm, M.D. Allendorf, B.C. Wood, and F. El Gabaly, “Identifying the role of dynamic surface hydroxides in the dehydrogenation of Ti-doped $NaAlH_4$,” *ACS Appl. Mater. Interfaces* **11**, 4930 (2019).
6. A. Schneemann, J.L. White, S. Kang, S. Jeong, L.F. Wan, E.S. Cho, T.W. Heo, D. Prendergast, J.J. Urban, B.C. Wood, M.D. Allendorf, and V. Stavila, “Nanostructured metal hydrides for hydrogen storage,” *Chem. Rev.* **118**, 10775 (2018).
7. M.D. Allendorf, Z. Hulvey, T. Gennett, T. Autrey, J. Camp, H. Furukawa, M. Haranczyk, M. Head-Gordon, A. Karkamkar, D.-J. Liu, J.R. Long, K. Meihaus, I. Nayyar, R. Narazov, D. Siegel, V. Stavila, J.J. Urban, S. Veccham, and B.C. Wood, “An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage,” *Energy Environ. Sci.* **11**, 2784 (2018).

Publications

8. S. Kang, L.E. Klebanoff, A.A. Baker, D.F. Cowgill, V.N. Stavila, M.D. Allendorf, J.R.I. Lee, M.H. Nielsen, K.G. Ray, Y.-S. Liu, and B.C. Wood*, "Assessing the reactivity of $TiCl_3$ and TiF_3 with hydrogen," *Int. J. Hydrogen Energy* **43**, 14507 (2018).
9. X.W. Zhou, T.W. Heo, B.C. Wood, S. Kang, M.D. Allendorf, and V. Stavila, "Molecular dynamics studies of fundamental bulk properties of palladium hydrides for hydrogen storage," *J. Appl. Phys.* **123**, 225105 (2018).
10. W.A. Braunecker, K.E. Hurst, K.G. Ray, Z.R. Owczarczyk, M.B. Martinez, A. Keuhlen, A. Sellinger, J.C. Johnson, "Phenyl/perfluorophenyl stacking interactions enhance structural order in two-dimensional covalent organic frameworks," *Cryst. Growth Des.* **18**, 4160 (2018).
11. S. Turner, W. Yan, H. Long, A.J. Nelson, A. Baker, J.R. Lee, C. Carraro, W.A. Worsley, R. Maboudian, and A. Zettl, "Boron doping and defect engineering of graphene aerogels for ultrasensitive NO_2 detection," *J. Phys. Chem. C* **122**, 20358.

Presentations

1. B.C. Wood, “Understanding frustration, correlation, and disorder in materials for energy storage and conversion,” Ecole Polytechnique Federal de Lausanne, Lausanne, Switzerland, May 2018.
2. B.C. Wood, “Predicting properties of complex interfaces for energy storage by integrating ab initio simulations with high-fidelity experiments,” American Chemical Society Meeting, Boston, MA, August 2018 [invited].
3. S. Kang, “Modeling of hydrogen storage materials using first-principles calculations,” US-Korea Conference (UKC), New York, NY, August 2018.
4. L. Wan, “Integrated experiment-theory approach to elucidate complex surface and interfacial chemistry in hydrogen storage materials,” Molecular Foundry User Meeting, Berkeley, CA, August 2018 [poster].
5. B.C. Wood, “Understanding reactive interfaces in complex metal hydrides through multiscale simulations,” 16th International Symposium on Metal-Hydrogen Systems, Guangzhou, China, October 2018 [invited].
6. S. Kang, “First-Principles Modeling of Hydrogen Storage Materials,” Korea Research Institute of Standards and Science (KRISS), Daejeon, Korea, October 2018.
7. B.C. Wood, “Modeling kinetic mechanisms governing hydrogen interactions with complex hydrides,” Korea Advanced Institute of Science and Technology, Daejeon, Korea, October 2018.
8. S. Kang, “Advanced modeling of thermodynamics in complex metal hydrides for hydrogen storage,” Korea Advanced Institute of Science and Technology, Daejeon, Korea, October 2018.
9. T.W. Heo, “HyMARC mesoscale modeling efforts for metal hydrides,” Korea Advanced Institute of Science and Technology, Daejeon, Korea, October 2018.
10. B.C. Wood, “Hydrogen materials research at the U.S. Department of Energy: A high-performance computing perspective,” Hyundai Motors Hydrogen Energy Development Team, Seoul, Korea, October 2018.

Presentations

11. B.C. Wood, “Atomic-scale computational studies of metal hydrides within the HyMARC Consortium,” Helmholtz-Zentrum Geesthacht, Germany, December 2018.
12. S. Kang, “Multiscale Simulations of Entropy and Phase Nucleation in the Mg-B-H System,” 13th International Symposium on Hydrogen & Energy, Incheon, Korea, January 2019.
13. T.W. Heo, “HyMARC mesoscale modeling efforts for metal hydrides,” Helmholtz-Zentrum Geesthacht, Germany, December 2018.
14. B.C. Wood, “Probing complex interfaces for renewable production and storage of hydrogen,” San Francisco State University, February 2019.