U.S. DEPARTMENT OF ENERGY
Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Hydrogen Materials Advanced Research Consortium (HyMARC)

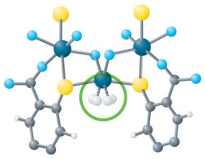
HyMARC Hydrogen Materials Advanced Research Consortium

Enabling **twice the energy density** for hydrogen storage

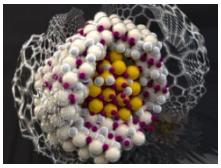
HyMARC is a National Lab-led consortium working to advance and develop hydrogen storage materials that meet DOE targets for energy density, kinetics, and cost. EERE's Hydrogen and Fuel Cell Technologies Office launched HyMARC in 2015 bringing together world-class National Lab capabilities in materials modelling, characterization, and synthesis; and fostering collaboration with industry and academia to overcome R&D challenges in materials-based hydrogen storage. HyMARC's main goal is to enable hydrogen storage materials with ***twice the energy density*** over current hydrogen storage technologies.

ACCOMPLISHMENTS

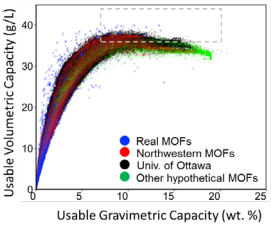
- **Demonstrated pathways to higher H_2 densities** with the first material which binds two H_2 molecules at a metal-organic framework (MOF) open metal site; and with a vanadium-based MOF that is the first material with an adsorption enthalpy within the 15-25 kJ/mol range predicted to enable room temperature operation (21 kJ/mol), and a 101% higher usable gravimetric capacity compared to the MOF-5 benchmark (-40°C to 25°C/5 to 100 bar).



- **Identified synthetic routes to improved operation conditions** for the promising $Mg(BH_4)_2$ system by 100°C and 200 bar lower than prior state of the art, and found that the addition of an electrolyte facilitates a 10x improvement of dehydrogenation kinetics.



- **Developed new formats of metal hydrides with improved properties**, demonstrating doubled hydrogenation and dehydrogenation rates of Li_3N through confinement within nanoporous carbon structures; simulations used to improve mechanistic understanding of the underlying processes.
- **Applied machine learning and computational modeling techniques** to screen 500,000+ real and hypothetical structures for usable capacities; thousands were identified with the potential to outperform current state-of-the-art MOFs.



EXAMPLES OF HYMARC CAPABILITIES

- A world-class adsorption measurement validation facility
- Full suite of neutron and X-ray characterization techniques
- In-situ, variable pressure DRIFTS, NMR, calorimetry
- Nanoscale material synthesis
- Comprehensive set of modeling and simulation tools
- System modeling and techno-economic analysis

ORGANIZATION

Five national labs make up HyMARC's core team

NREL National Renewable Energy Laboratory
Sandia National Laboratories
Pacific Northwest National Laboratory
Berkeley Lab
Lawrence Livermore National Laboratory

Streamlined access to several lab user facilities

ALS Advanced Light Source
SNS Spallation Neutron Source
NIST Center for Neutron Research
Molecular Foundry
SLAC National Accelerator Laboratory

The core lab group works synergistically with new seedling projects solicited through funding opportunity announcements (20 projects to date—*full list on page 2*).

HyMARC by the Numbers

130+ publications and 1 book chapter
9 patents and 2 pending
60+ lab staff/scientists
57 postdocs
35 grad students
13 undergrads involved

Contacts

For more information about HyMARC, visit their website, **hymarc.org**, or contact the co-directors: **Mark Allendorf** (mdallen@sandia.gov) and **Tom Gennett** (Thomas.Gennett@nrel.gov)

For more information, visit:
hydrogenandfuelcells.energy.gov

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Leadership, Tasks, and Focus Areas

HyMARC Directors

Mark Allendorf (SNL)
Tom Gennett (NREL)

Core Lab Leads

Tom Autrey (PNNL)
Jeff Long (LBNL)
David Prendergast (LBNL)
Vitalie Stavila (SNL)
Brandon Wood (LLNL)

Task 1: Sorbents

- Enthalpy/entropy
- Optimization of binding energies
- Sorbent packing
- Dynamic sorbents
- Multiple H_2 binding
- Nanoscale defects

Task 2: Hydrides

- Metal hydride thermodynamics
- Solid interfaces and surfaces
- Activation of B-B and B-H bonds
- Nanoscaling to improve thermo/kinetics
- Microstructural impacts
- Machine learning for new MH

Task 3: Carriers

- Alternate electrochemical approaches
- Priorities for liquid organic H_2 carriers
- Eutectic systems as carriers
- Adsorbents as carriers
- Bioinspired carriers
- Catalyst stability
- Plasmon interactions for release
- Heterolytic cleavage and activation

Task 4: Advanced Characterization

- High temp PCT system
- PCT calorimetry
- Advanced NMR
- Neutron/synchrotron and ATR DRIFTS

Task 5: Seedling Support

Task 6: Data Hub

HyMARC Individual Projects to Date

PROJECT TITLE	LOCATION
Development of Magnesium Boride Etherates as Hydrogen Storage Materials	University of Hawaii at Manoa
Electrolyte Assisted Hydrogen Storage Reactions	Liox Power, Inc.
Optimized Hydrogen Adsorbents via Machine Learning and Crystal Engineering	University of Michigan
ALD (Atomic Layer Deposition) Synthesis of Novel Nanostructured Metal Borohydrides	National Renewable Energy Laboratory
Methane and Hydrogen Storage with Porous Cage-Based Composite Materials	University of Delaware
Optimal Adsorbents for Low-Cost Storage of Natural Gas: Computational Identification, Experimental Demonstration, and System-Level Projection	University of Michigan
Metal-Organic Frameworks Containing Frustrated Lewis Pairs for Hydrogen Storage at Ambient Temperature	University of South Florida
Heteroatom-Modified and Compacted Zeolite-Templated Carbons for Gas Storage	Montana State University
Developing a New NG Super-Adsorbent Polymer (NG-SAP) for a Practical NG Storage System with Low Pressure, Ambient Temperature, and high Energy Density	Penn State University
Uniting Theory and Experiment to Deliver Flexible MOFs for Superior Methane (NG) Storage	University of South Florida
Hydrogen Release from Concentrated Media with Reusable Catalysts	University of Southern California
Theory-Guided Design and Discovery of Materials for Reversible Methane and Hydrogen Storage	Northwestern University
High Capacity Step-Shaped Hydrogen Adsorption in Robust, Pore-Gating Zeolitic Imidazolate Frameworks	Colorado School of Mines
A Reversible Liquid Hydrogen Carrier System Based on Ammonium Formate and Captured CO2	Washington State University
Development of Magnesium Borane Containing Solutions of Furans and Pyrroles as Reversible Liquid Hydrogen Carriers	University of Hawaii at Manoa
Developing a Novel Hydrogen Sponge with Ideal Binding Energy and High Surface Area for Practical Hydrogen Storage (project complete)	Penn State University
Fundamental Studies of Surface-Functionalized Mesoporous Carbons for Thermodynamic Stabilization and Reversibility of Metal Hydrides (project complete)	University of Missouri-St. Louis
"Graphene-Wrapped" Complex Hydrides as High-Capacity, Regenerable Hydrogen Storage Materials (project complete)	Argonne National Laboratory
Super Metallated Frameworks as Hydrogen Sponges (project complete)	University of California, Berkeley
Fluorinated Covalent Organic Frameworks: A Novel Pathway to Enhance Hydrogen Sorption and Control Isosteric Heats of Adsorption (project complete)	National Renewable Energy Laboratory