Hydrogen Storage Materials Database Demonstration

12/13/2011

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Storage Tech Team Lead
Fuel Cell Technologies Program
U.S. Department of Energy

Hydrogen Storage Materials Database

www.bcs-hq.com

Marni Lenahan
December 13, 2011

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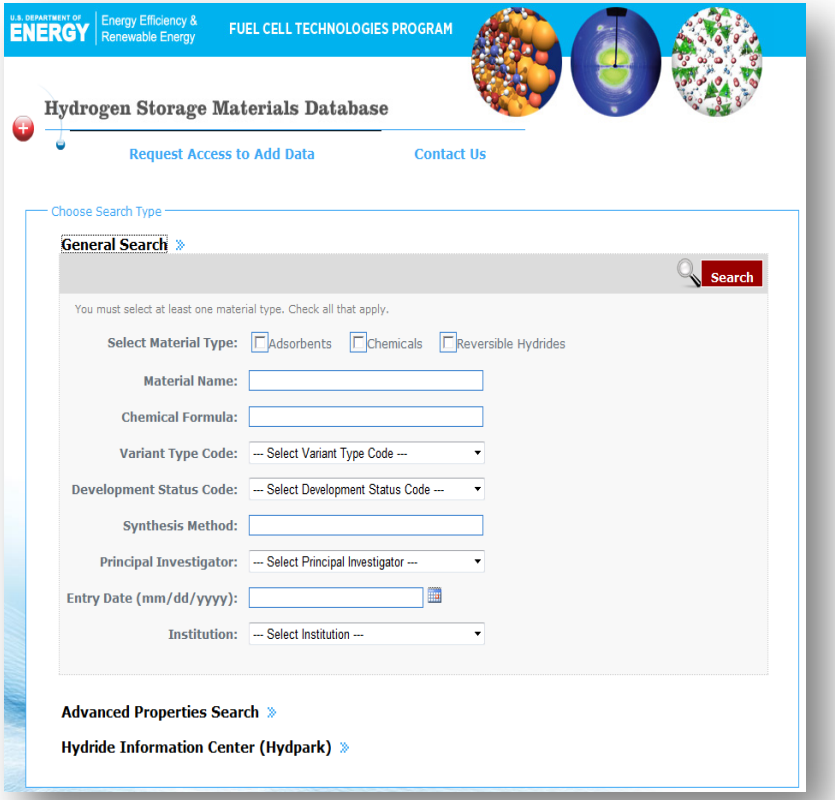
Database Background

- The Hydrogen Storage Materials Database was built to retain information from DOE Hydrogen Storage funded research and make these data more accessible.

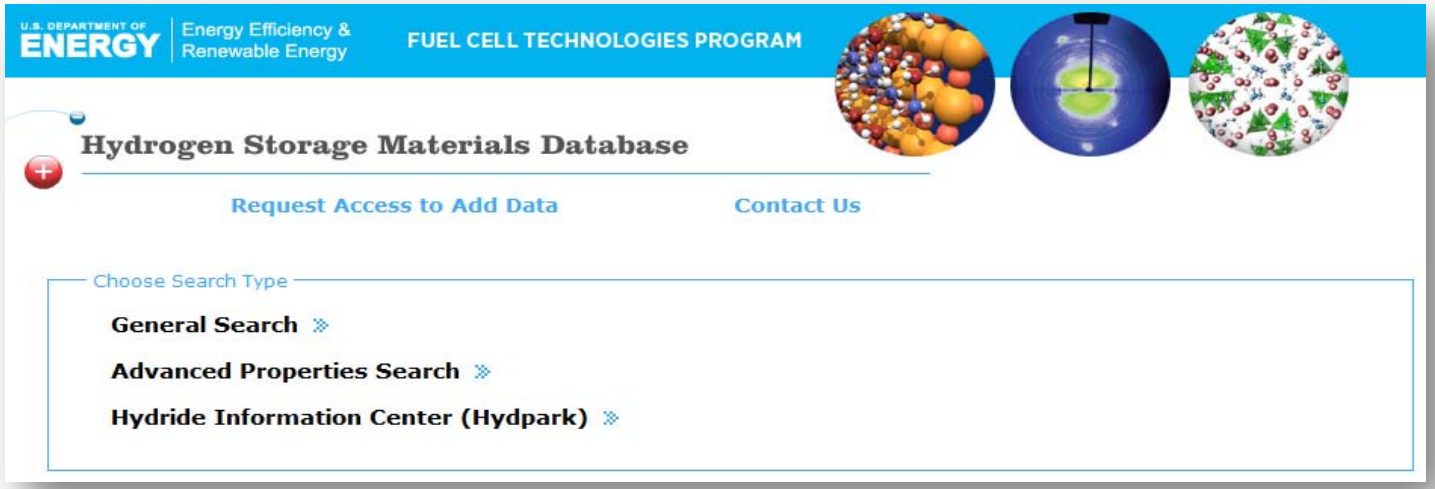
- Data includes properties of hydrogen storage materials investigated such as synthesis conditions, sorption and release conditions, capacities, thermodynamics, etc.



http://hydrogenmaterialssearch.govtools.us

Current Status

- Data continues to be collected from DOE funded research.
- The objective of this database is for it to be a resource for the research community to accelerate the development of advanced hydrogen storage materials.



Data Types

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Two Types of Data

Hydpark Data

- Historical data collection of metal-hydrogen systems including their properties, applications, and literature sources
- Funded by DOE and Sandia National Laboratories to contribute to IEA-HIA

Current Data

- Includes data from:
  - DOE funded research since 2002
  - Requestors, upon approval
- Categories of materials include:
  - Adsorbents
  - Chemical materials
  - Reversible Hydrides

Demonstration

Hydrogen Storage Materials Database

General Search Example: Ammonia Borane

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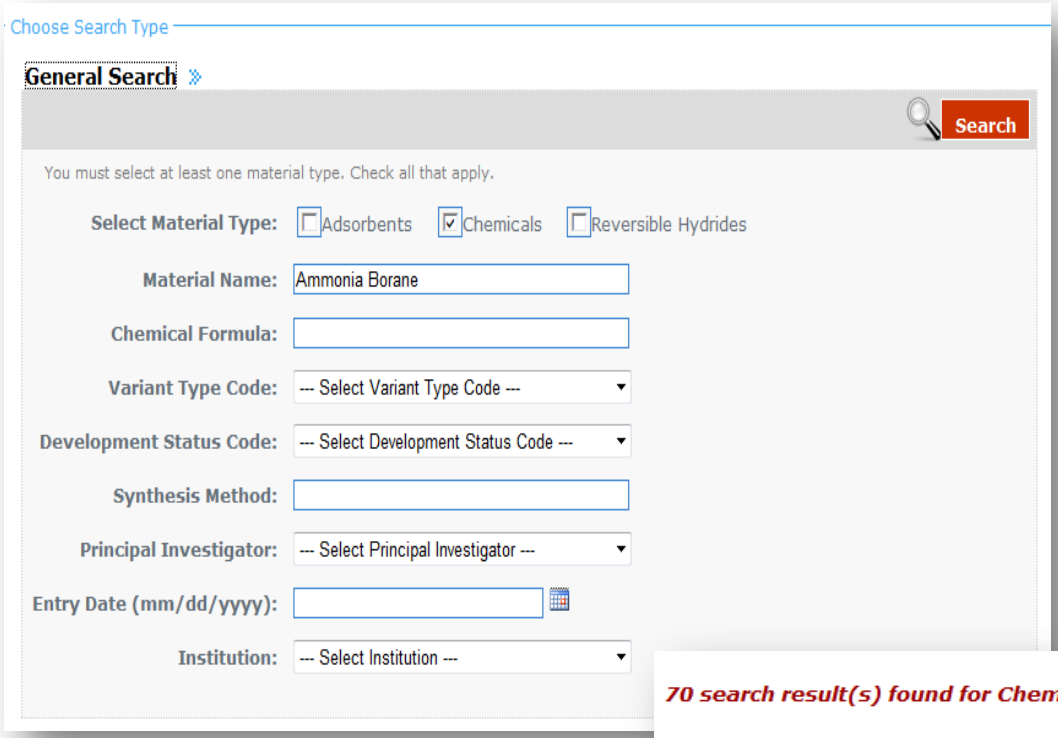

70 search result(s) found for Chemicals

Show Details

Material Name	Chemical Formula	Principal Investigator	Institution
Ammonia Borane (Show Details)	NH3BH3	Kevin Ott	University Of Washington
Ammonia Borane (AB) (Show Details)	NH3BH3	Abhi Karkamkar	Pacific Northwest National Laboratory
Ammonia Borane (AB) + Ammonium chloride (Show Details)	NH3BH3+NH3Cl (20%)		Pacific Northwest National Laboratory

Detailed Information

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Hide Details

Material Name	Chemical Formula	Principal Investigator	Institution	Variant Type Code	Development Status Code	Synthesis Method	Synthesis Conditions	Precursors	Activation	Entry Date	H Weight Density Theory (theoretical wt%)	H Weight Density Experiment (observed wt%)	H Weight Density Reference	H Volume Density Theory (g/L)
[illegible] (Show Details)	NH3BH3	Kevin Ott	University Of Washington	Homogeneous Catalyst	Discontinued Development		Conventional organometallic synthesis methods			11/21/2011	19.40	6.50	B. L. Dietrich et al, J. Am. Chem. Soc. 2008, 47, 8583.	
Ammonia Borane (AB) (Show Details)	NH3BH3	Abhi Karkamkar	Pacific Northwest National Laboratory	Other (OT2)	Discontinued Development	Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160.				03/29/2011	19.40	16.00		146.00
Ammonia Borane (AB) + Ammonium chloride (Show Details)	NH3BH3+NH3Cl (20%)		Pacific Northwest National Laboratory	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive	N/A	N/A	N/A	02/02/2011				

Detail Information

Material Name: Ammonia Borane
Chemical Formula: NH3BH3
Principal Investigator: Kevin Ott
Institution: University Of Washington
Variant Type Code: Homogeneous Catalyst
Development Status Code: Discontinued Development
Synthesis Method:
Synthesis Conditions: Conventional organometallic synthesis methods
Synthesis Method Reference:
Precursors:
Activation:
Entry Date: 11/21/2011
H Weight Density Theory (theoretical wt%): 19.40
H Weight Density Experiment (observed wt%): 6.50
H Weight Density Reference: B. L. Dietrich et al, J. Am. Chem. Soc. 2008, 47, 8583.
H Volume Density Theory (g/L):
H Volume Density Experiment (g/L):
H Volume Density Reference (g/L):
Temperature Onset Release (k): 300
Impurities Released: Low temperature release, none detected
Temperature FullRelease (k): 298
Temperature Release Reference: B. L. Dietrich et al, J. Am. Chem. Soc. 2008, 47, 8583.
Additional Comments:

Close Window

Two Ways to Display Additional Details

Export Data

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General Search Result

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General Search Result

70 search result(s) found for Chemicals

Item No.	Material Name	Chemical Formula	Variant Type Code	Development Status Code	Synthesis Method
1	Ammonia Borane	NH3BH3	Homogeneous Catalyst	Discontinued Development	
2	Ammonia Borane (AB)	NH3BH3	Other (OT2)	Discontinued Development	Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160.
3	Ammonia Borane (AB) + Ammonium chloride	NH3BH3+NH3Cl (20%)	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive
4	Ammonia Borane (AB) + beta-cyclodextin	30wt% beta-cyclodextin	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive
5	Ammonia Borane (AB) + boric acid	30 wt% boric acid	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive
6	Ammonia Borane (AB) + Cellulose	30 wt% and 50 wt%	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive
7	Ammonia Borane (AB) + Citric acid	30 wt% citric acid	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive
8	Ammonia Borane (AB) + d-glucose	30wt% additive	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive
9	Ammonia Borane (AB) + Dextrin	30wt% additive	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive
10	Ammonia Borane (AB) + diethylene glycol	10, 29 wt% additive	Other (OT2)	Discontinued Development	AB by Heldebrant, D.J., et al., Energy & Environmental Science, 2008. 1(1): p. 156-160. plus ball milling of additive

Advanced Search: Institution

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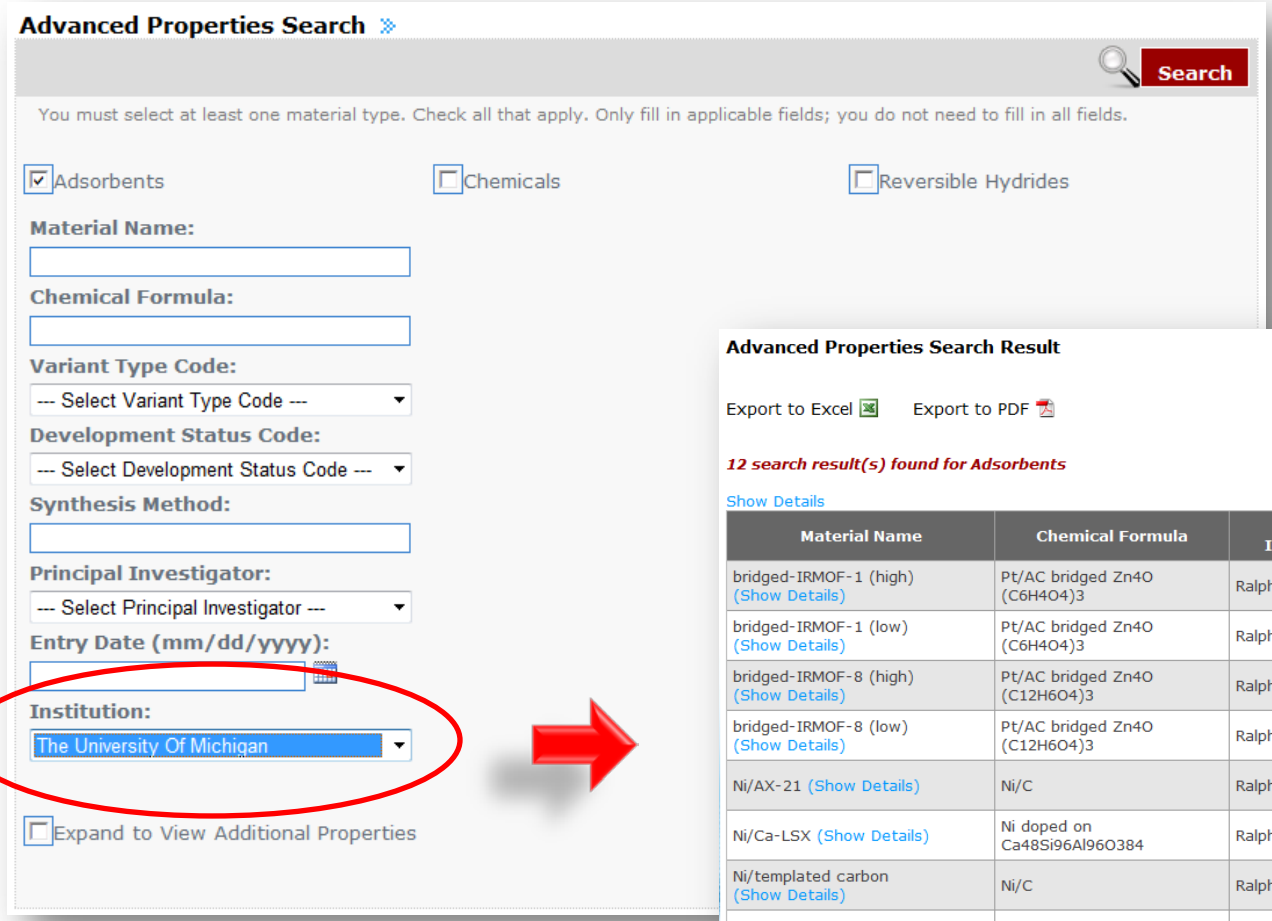

Advanced Properties Search Result

Export to Excel Export to PDF

12 search result(s) found for Adsorbents

Show Details

Material Name	Chemical Formula	Principal Investigator	Institution
bridged-IRMOF-1 (high) (Show Details)	Pt/AC bridged Zn4O (C6H4O4)3	Ralph Yang	The University Of Michigan
bridged-IRMOF-1 (low) (Show Details)	Pt/AC bridged Zn4O (C6H4O4)3	Ralph Yang	The University Of Michigan
bridged-IRMOF-8 (high) (Show Details)	Pt/AC bridged Zn4O (C12H6O4)3	Ralph Yang	The University Of Michigan
bridged-IRMOF-8 (low) (Show Details)	Pt/AC bridged Zn4O (C12H6O4)3	Ralph Yang	The University Of Michigan
Ni/AX-21 (Show Details)	Ni/C	Ralph Yang	The University Of Michigan
Ni/Ca-LSX (Show Details)	Ni doped on Ca48Si96Al96O384	Ralph Yang	The University Of Michigan
Ni/templated carbon (Show Details)	Ni/C	Ralph Yang	The University Of Michigan
Pt/AX-21 (Show Details)	Pt/C	Ralph Yang	The University Of Michigan
Pt/Ca-LSX (Show Details)	Pt doped on Ca48Si96Al96O384	Ralph Yang	The University Of Michigan
Pt/templated carbon (Show Details)	Pt/C	Ralph Yang	The University Of Michigan
Ru/AX-21 (Show Details)	Ru/C	Ralph Yang	The University Of Michigan
Ru/templated carbon (Show Details)	Ru/C	Ralph Yang	The University Of Michigan

Advanced Search: Primary Investigator

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Advanced Properties Search

Search

You must select at least one material type. Check all that apply. Only fill in applicable fields; you do not need to fill in all fields.

- [ ] Adsorbents
- [x] Chemicals
- [ ] Reversible Hydrides

Material Name:

Chemical Formula:

Variant Type Code: --- Select Variant Type Code ---

Development Status Code: --- Select Development Status Code ---

Synthesis Method:

Principal Investigator: Sneddon, Larry

Entry Date (mm/dd/yyyy):

Institution: --- Select Institution ---

- [ ] Expand to View Additional Properties

15 search result(s) found for Chemicals

Show Details

Material Name	Chemical Formula	Principal Investigator	Institution
AB/bmimCl(20wt%)-1 (Show Details)	H3NBH3/bmimCl(20wt%)-1	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(20wt%)-2 (Show Details)	H3NBH3/bmimCl(20wt%)-2	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)-1 (Show Details)	H3NBH3/bmimCl(50wt%)-1	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)-2 (Show Details)	H3NBH3/bmimCl(50wt%)-2	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)-3 (Show Details)	H3NBH3/bmimCl(50wt%)-3	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)-4 (Show Details)	H3NBH3/bmimCl(50wt%)-4	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)/PS(1mol%)-1 (Show Details)	H3NBH3/bmimCl(50wt%)/PS (1mol%)-1	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)/PS(1mol%)-2 (Show Details)	H3NBH3/bmimCl(50wt%)/PS (1mol%)-2	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)/PS(5mol%)-1 (Show Details)	H3NBH3/bmimCl(50wt%)/PS (5mol%)-1	Larry Sneddon	University Of Pennsylvania
AB/bmimCl(50wt%)/PS(5mol%)-2 (Show Details)	H3NBH3/bmimCl(50wt%)/PS (5mol%)-2	Larry Sneddon	University Of Pennsylvania
AB/PS(5mol%) (Show Details)	H3NBH3/PS(5mol%)	Larry Sneddon	University Of Pennsylvania
AB/tetraglyme(50wt%) (Show Details)	H3NBH3/tetraglyme(50wt%)	Larry Sneddon	University Of Pennsylvania
AB/tetraglyme(50wt%)/PS(1mol%) (Show Details)	H3NBH3/tetraglyme (50wt%)/PS(1mol%)	Larry Sneddon	University Of Pennsylvania
AB/tetraglyme(50wt%)/PS(5mol%) (Show Details)	H3NBH3/tetraglyme (50wt%)/PS(5mol%)	Larry Sneddon	University Of Pennsylvania
DADB/bmimCl(50wt%) (Show Details)	(BH2(NH3)2)BH4/bmimCl (50wt%)	Larry Sneddon	University Of Pennsylvania

Advanced Search: Reversible Hydrides

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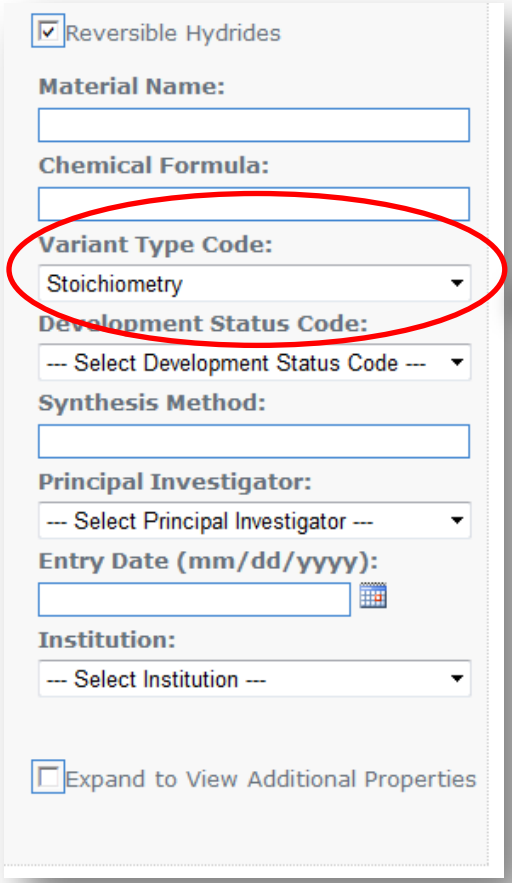

15 search result(s) found for Reversible Hydrides

Show Details

Material Name	Chemical Formula	Principal Investigator	Institution
alpha aluminum hydride (Show Details)	alpha-AlH3	Jason Graetz	Brookhaven National Laboratory
Alumino borane (Show Details)	AlB6H13	J. C. Zhao	Ohio State University
Aluminoborane (Show Details)	Al(BH4)3 + B10H14	J. C. Zhao	Ohio State University
aluminoborane (Show Details)	AlB4H11	J. C. Zhao	Ohio State University
beta aluminum hydride (Show Details)	beta-AlH3	Jason Graetz	Brookhaven National Laboratory
Calcium aluminum hydride (Show Details)	Ca(AlH4)2	Jason Graetz	Brookhaven National Laboratory
Dimethylethylamine alane (Show Details)	C4H11N-AlH3	Jason Graetz	Brookhaven National Laboratory
gamma aluminum hydride (Show Details)	gamma-AlH3	Jason Graetz	Brookhaven National Laboratory
Hexamine alane (Show Details)	C6H12N4-AlH3	Jason Graetz	Brookhaven National Laboratory
potassium lithium aluminum hydride (Show Details)	K2LiAlH6	Jason Graetz	Brookhaven National Laboratory
potassium sodium aluminum hydride (Show Details)	K2NaAlH6	Jason Graetz	Brookhaven National Laboratory
Quinuclidine alane (Show Details)	2C7H13N-AlH3	Jason Graetz	Brookhaven National Laboratory
sodium lithium aluminum hydride (Show Details)	Na2LiAlH6	Jason Graetz	Brookhaven National Laboratory
Triethylenediamine alane (Show Details)	C6H12N2-AlH3	Jason Graetz	Brookhaven National Laboratory
Trimethylamine alane (Show Details)	2C3H9N-AlH3	Jason Graetz	Brookhaven National Laboratory

Hydride Information Center Example: A2B

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Hydride Information Center (Hydpark)

Search

Material Class:	A2B			
Composition Formula:				
Hydrogen Weight Percent:	Min:		Max:	
Heat of Formation (kJ/mol H2):	Min:		Max:	
Temperature (°C):	Min:	100	Max:	300
Pressure (Atmospheres Absolute):	Min:		Max:	
Author:	--- Select Author ---			
Year:	--- Select Year ---			

HydPark Data Overview

140 search result(s) found

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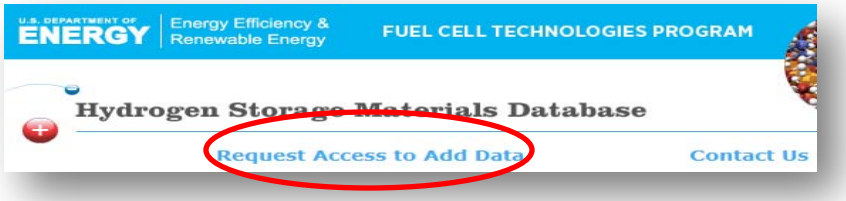
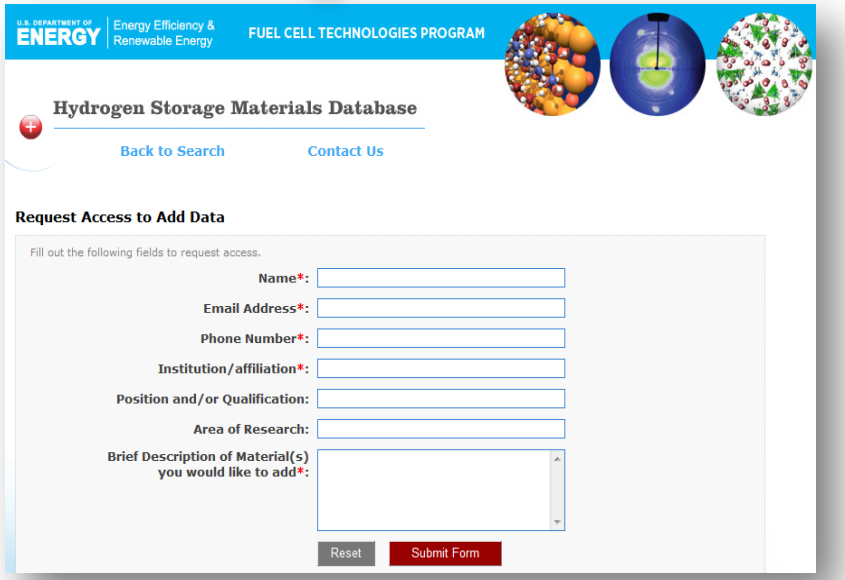
Material Class	Composition Formula	Hydrogen Weight Percent	Heat of Formation (kJ/mol H2)	Temperature (°C)	Pressure (Atmospheres Absolute)	Author Year	Reference Number	Comment1
A2B	Mg2Ni1-yBey	3.9	71 - 80	337	3 - 5	Lupu, 1982	419	(y = 0.15-0.25)
A2B	Mg2Ni1-yCuy	2.6	53 - 73	300	3.5 - 8	Darnaudery, 1983	417	(y = 0-1)
A2B	Pr2Al	1.4				Semenenko, 1985	1151	
A2B	Th1.5Ce.5Al	0.4	133	650	0.0003	Van Vucht, 1963	492	
A2B	Th2Al	0.8	130	500	0.001	Van Vucht, 1963	492	

Adding Data

- Select “Request Access to Add Data” at top of database on the homepage.
- Fill out required fields on the form and optional fields, if desired.
- The Database Administrator will send an e-mail notification to acknowledge receipt of the request and provide next steps.





Data Approval

- All data requests will be submitted to the Fuel Cell Technologies Program for approval.
- The Database Administrator will send the Requestor notification of approval and a spreadsheet for the Requestor to fill in with data.
- After the Database Administrator receives the data, the Database Administrator will provide the Requestor with estimated date for upload.
- All data will undergo a review to check for errors before being posted on the public site.

Next Steps

- Continue to collect data from Primary Investigators and other hydrogen storage research groups for incorporation into the database.
- Obtain feedback from users to further improve and enhance the functionality and usefulness of the database.
- Investigate opportunities to link the database to other data clearinghouses, such as Lawrence Berkeley National Laboratory's Materials Project (https://www.materialsproject.org/).

Questions?

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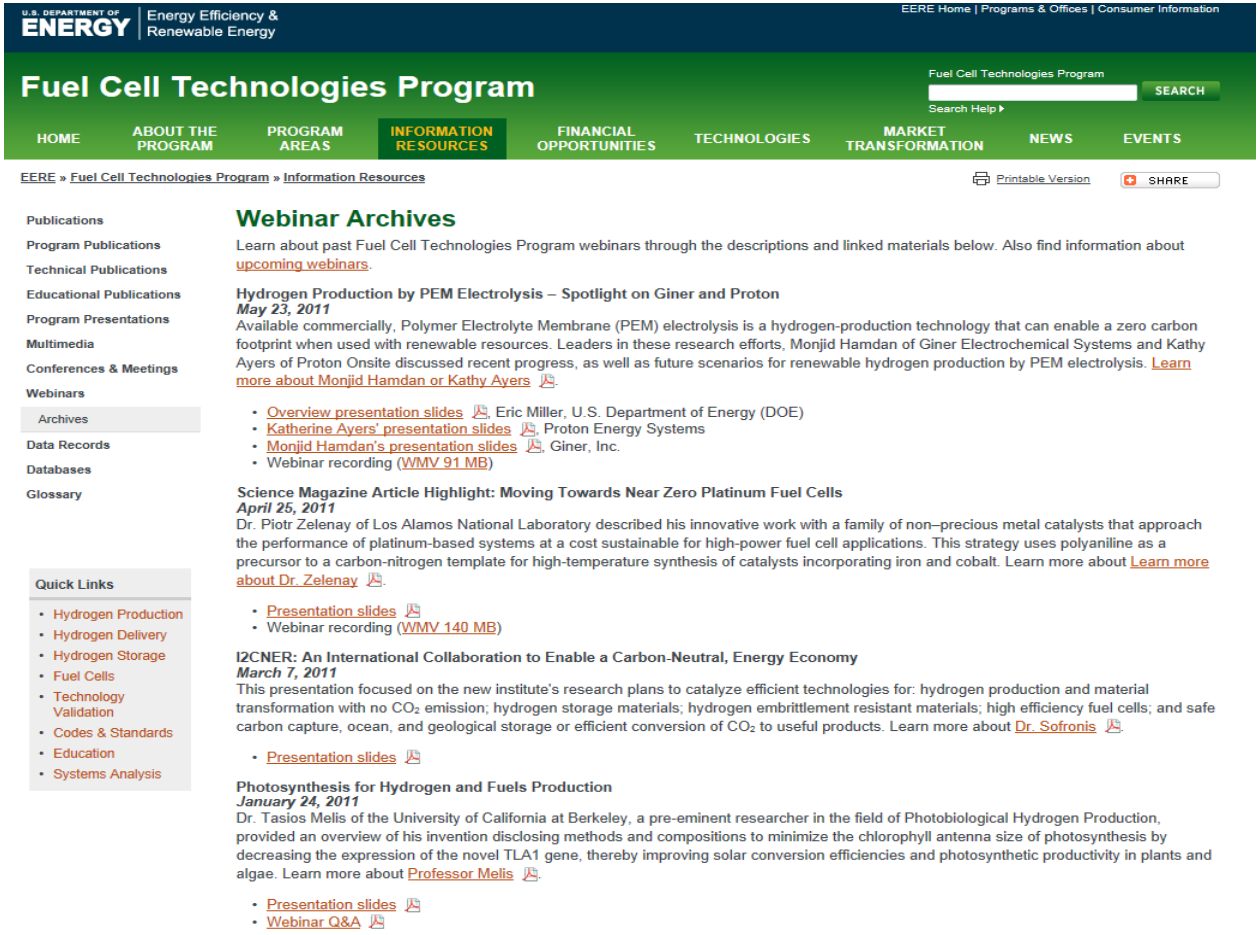
mlenahan@bcs-hq.com

Access the Hydrogen Storage Materials Database:

http://hydrogenmaterialssearch.govtools.us/

Slides from Previous Webinars



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Webinar Archives

Learn about past Fuel Cell Technologies Program webinars through the descriptions and linked materials below. Also find information about upcoming webinars.

Hydrogen Production by PEM Electrolysis – Spotlight on Giner and Proton
May 23, 2011
Available commercially, Polymer Electrolyte Membrane (PEM) electrolysis is a hydrogen-production technology that can enable a zero carbon footprint when used with renewable resources. Leaders in these research efforts, Monjid Hamdan of Giner Electrochemical Systems and Kathy Ayers of Proton Onsite discussed recent progress, as well as future scenarios for renewable hydrogen production by PEM electrolysis. Learn more about Monjid Hamdan or Kathy Ayers.

- Overview presentation slides, Eric Miller, U.S. Department of Energy (DOE)
- Katherine Ayers' presentation slides, Proton Energy Systems
- Monjid Hamdan's presentation slides, Giner, Inc.
- Webinar recording (WMV 91 MB)

Science Magazine Article Highlight: Moving Towards Near Zero Platinum Fuel Cells
April 25, 2011
Dr. Piotr Zelenay of Los Alamos National Laboratory described his innovative work with a family of non–precious metal catalysts that approach the performance of platinum-based systems at a cost sustainable for high-power fuel cell applications. This strategy uses polyaniline as a precursor to a carbon-nitrogen template for high-temperature synthesis of catalysts incorporating iron and cobalt. Learn more about Learn more about Dr. Zelenay.

- Presentation slides
- Webinar recording (WMV 140 MB)

I2CNER: An International Collaboration to Enable a Carbon-Neutral, Energy Economy
March 7, 2011
This presentation focused on the new institute's research plans to catalyze efficient technologies for: hydrogen production and material transformation with no CO_2 emission; hydrogen storage materials; hydrogen embrittlement resistant materials; high efficiency fuel cells; and safe carbon capture, ocean, and geological storage or efficient conversion of CO_2 to useful products. Learn more about Dr. Sofronis.

- Presentation slides

Photosynthesis for Hydrogen and Fuels Production
January 24, 2011
Dr. Tasios Melis of the University of California at Berkeley, a pre-eminent researcher in the field of Photobiological Hydrogen Production, provided an overview of his invention disclosing methods and compositions to minimize the chlorophyll antenna size of photosynthesis by decreasing the expression of the novel TLA1 gene, thereby improving solar conversion efficiencies and photosynthetic productivity in plants and algae. Learn more about Professor Melis.

- Presentation slides
- Webinar Q&A

To access the slides from this and previous Webcasts, please visit:
http://www1.eere.energy.gov/hydrogenandfuelcells/webinar_archives.html