Hydrogen Storage (II)

The key to an efficient energy storage

- High pressure
- Cryogenic
- Chemical Hydrides
- Metal Hydrides
- Physical Sorption

Metal Hydrides

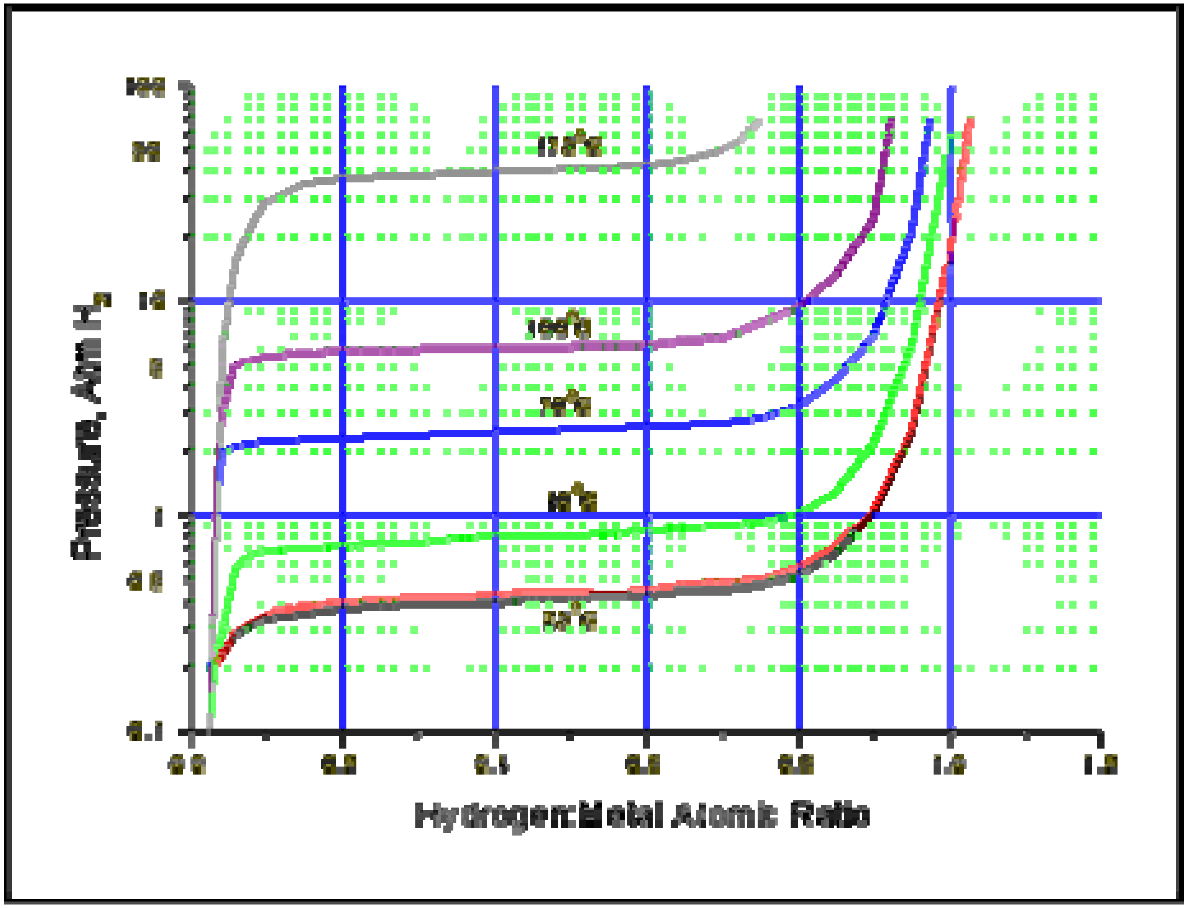
Simple metal hydrides

- Examples: NiH, PdH, $LaNi_5H_6$, MgH_2
- Metallic bond, H share mobile electrons with the metal atom
- Hydrogen mobility is generally high
- Gravimetric density from 1% ~ 8%
- Metal hydrides with lower H-content tend to have better reversibility

Simple Metal Hydrides: Classification

- AB_5 - $LaNi_5H_6$
- AB_2 - $ZnMn_2H_3$
- AB - $TiFeH_2$
- A_2B - Mg_2NiH_4
- Solid solution type -$V_{0.8}Ti_{0.2}$
- MgH_2 class (alkaline earth metal hydride)

Metal Hydrides: Isotherm

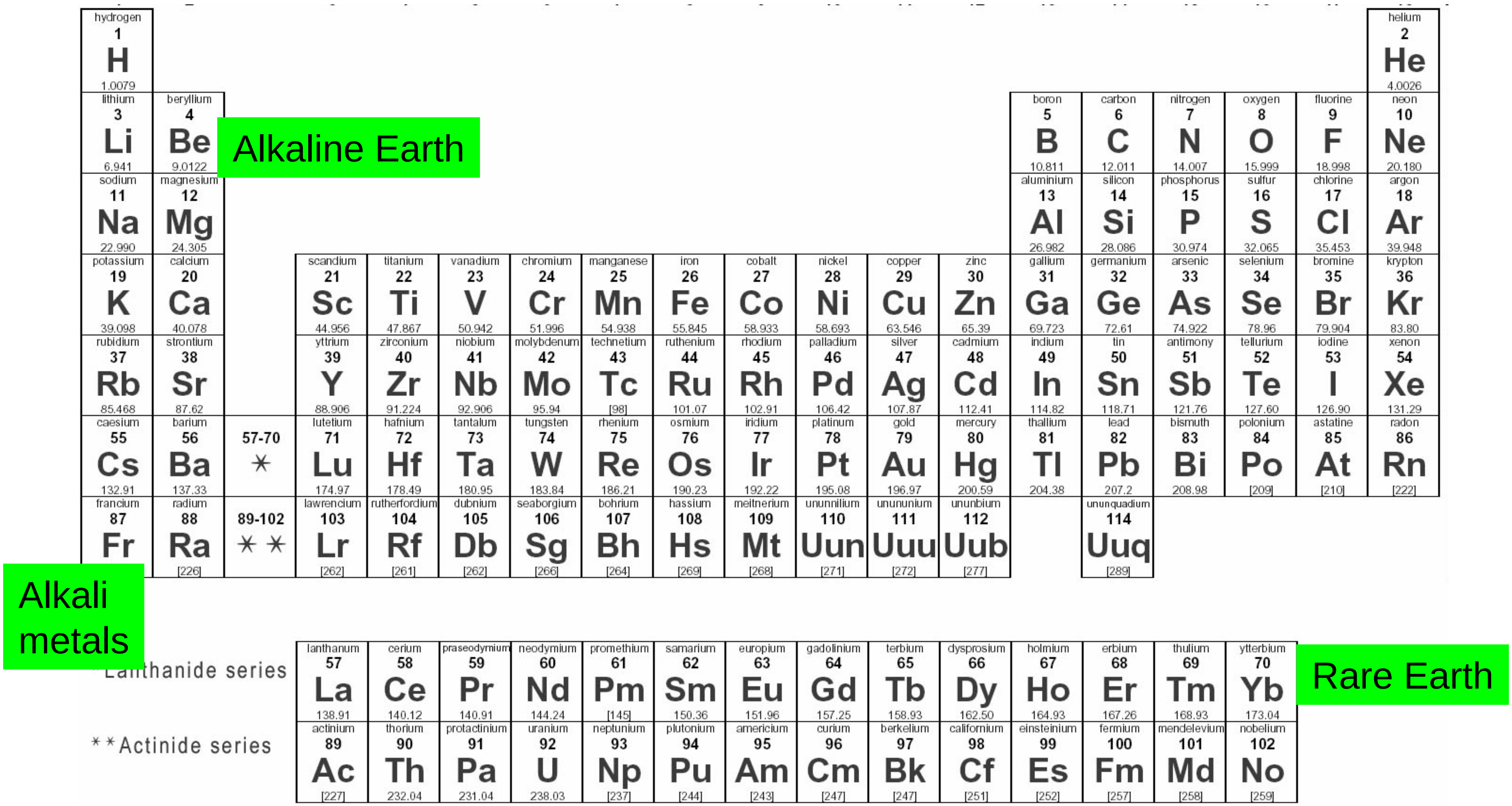


The isotherm tell us the working temperature and pressure of the hydride
And how much H it can store

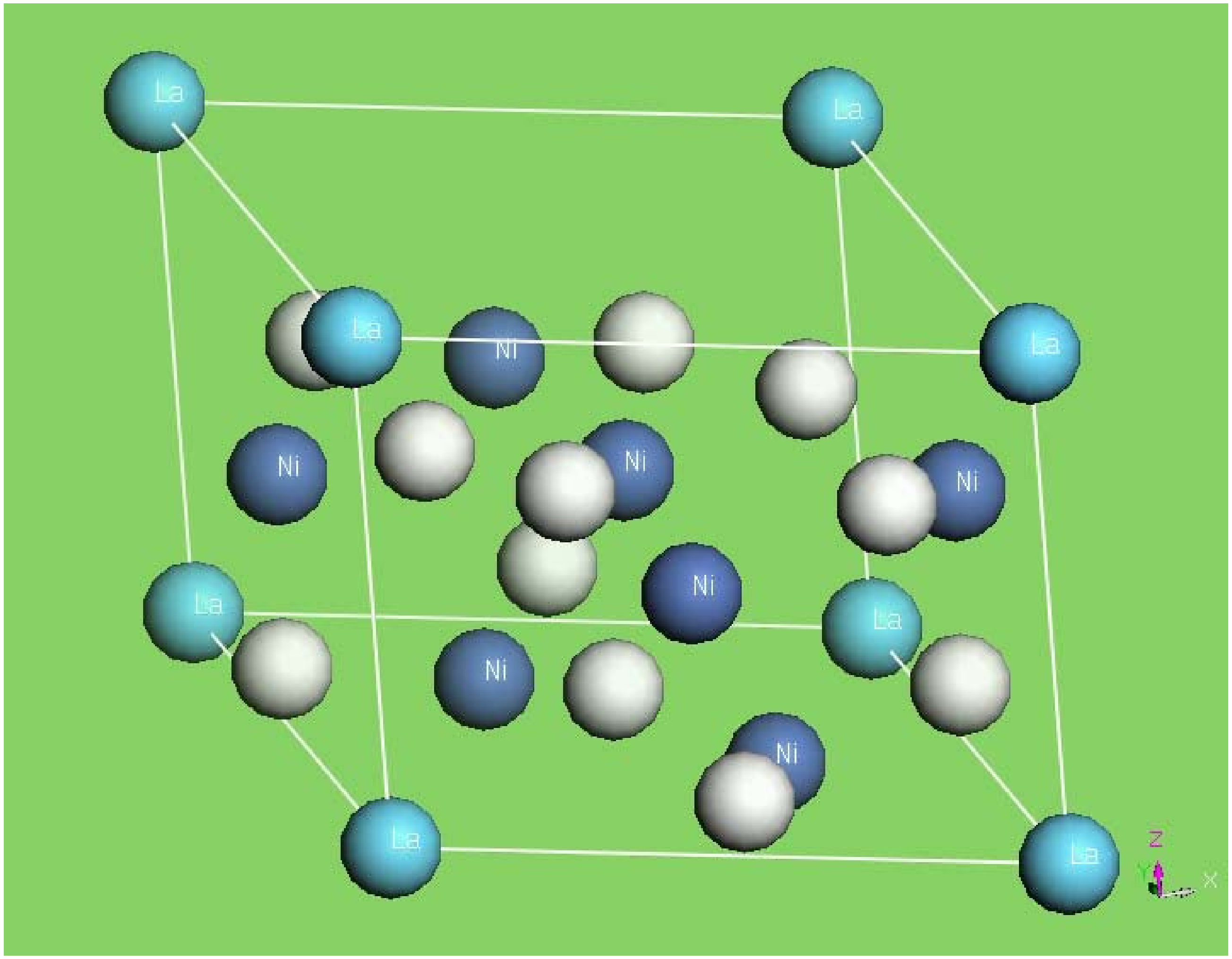
Metal Hydrides: $LaNi_5H_6$

- Most widely utilized MH today
- Gravimetric density ~ 1.3%-wt H
- Volumetric density ~ 0.1 kg/liter
- Cost high due to nickel, lanthanum (rare earth)
- Relative ease of refueling (near ambient pressure)
- It's the most representative AB_5 alloy
- Can be utilized in electrochemical cells (batteries and fuel cells) directly

The chemical elements



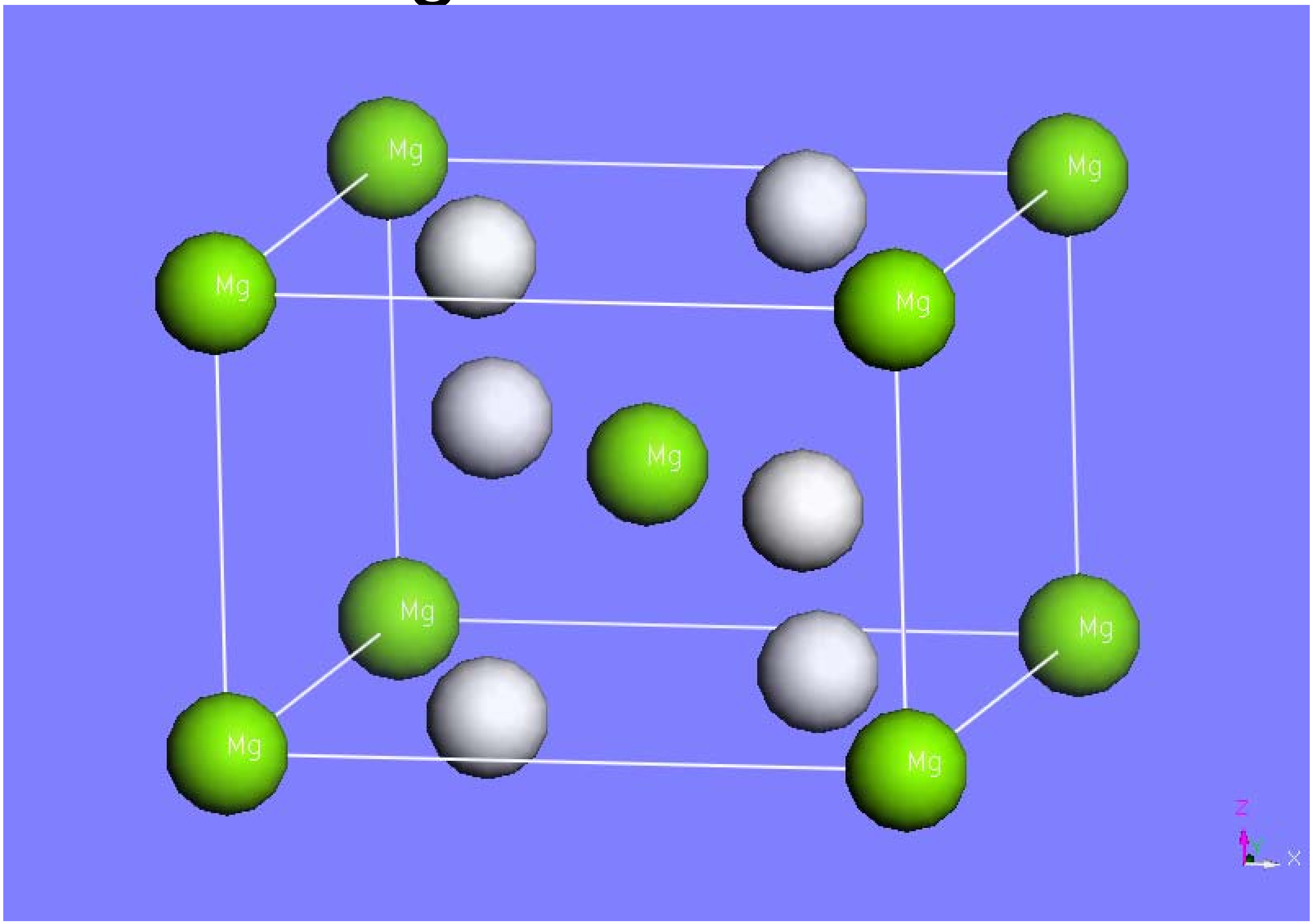
$LaNi_5H_6$: Structure



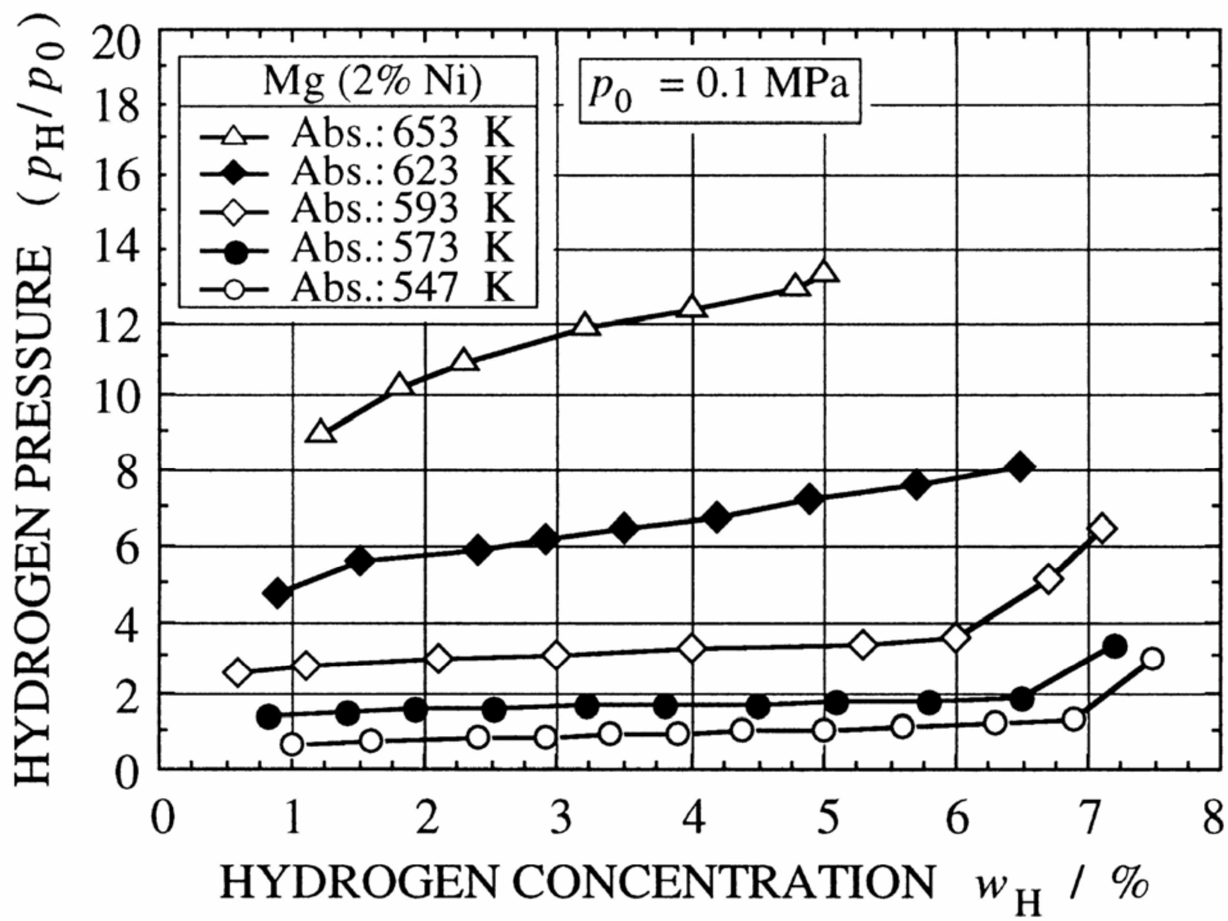
Metal Hydrides: MgH_2

- Gravimetric density ~ 8%-wt H
- Volumetric density >> 0.1 kg/liter
- Cost is low, very affordable
- Abundant element
- Clean
- Medium temperature absorption and de-sorption ~ 300 degrees C
- It’s the most representative alkaline earth metal hydride
- Not ideal for mobile H storage but ideal for stationary type applications

MgH_2: Structure



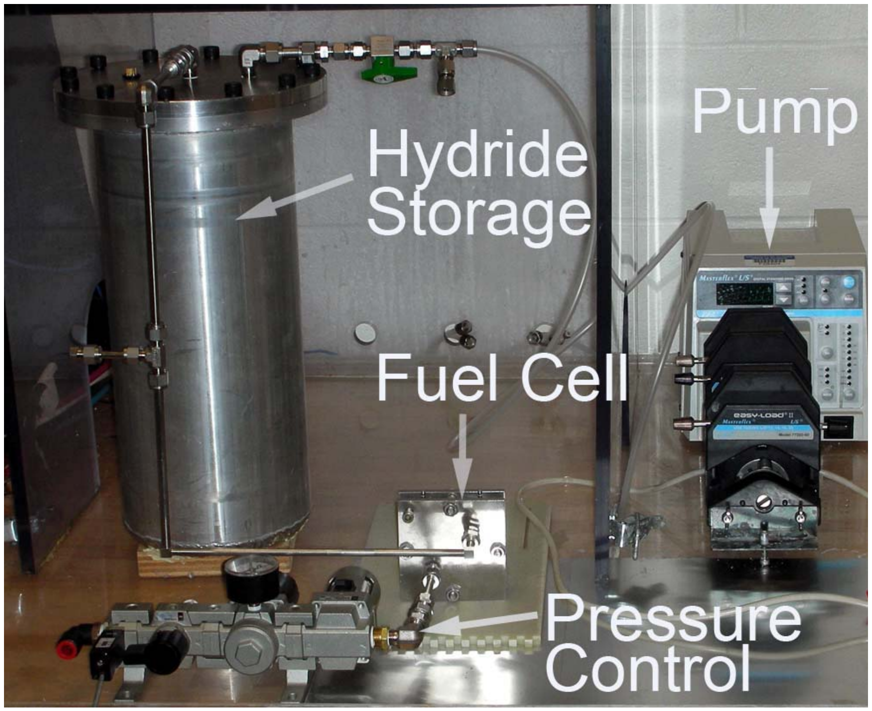
MgH_2: Isotherm

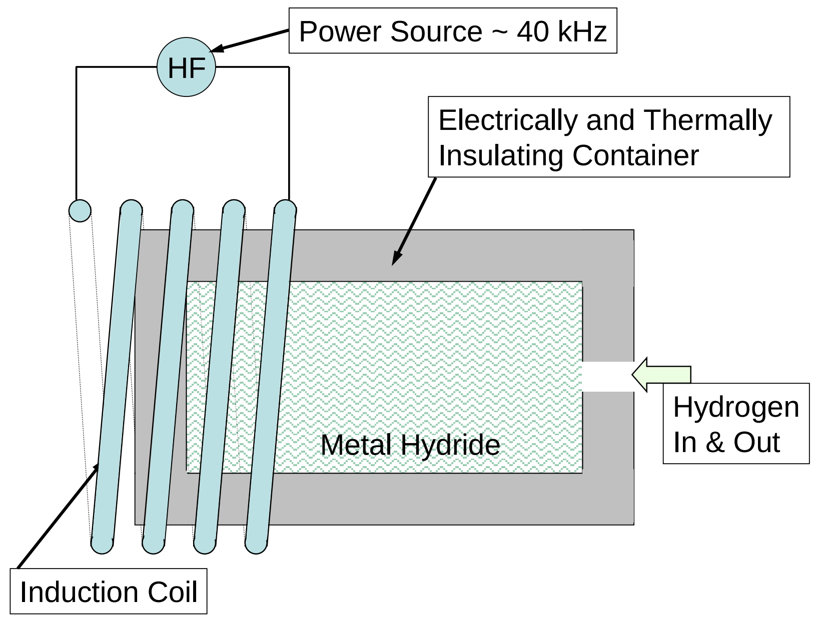


MgH_2: Kinetics

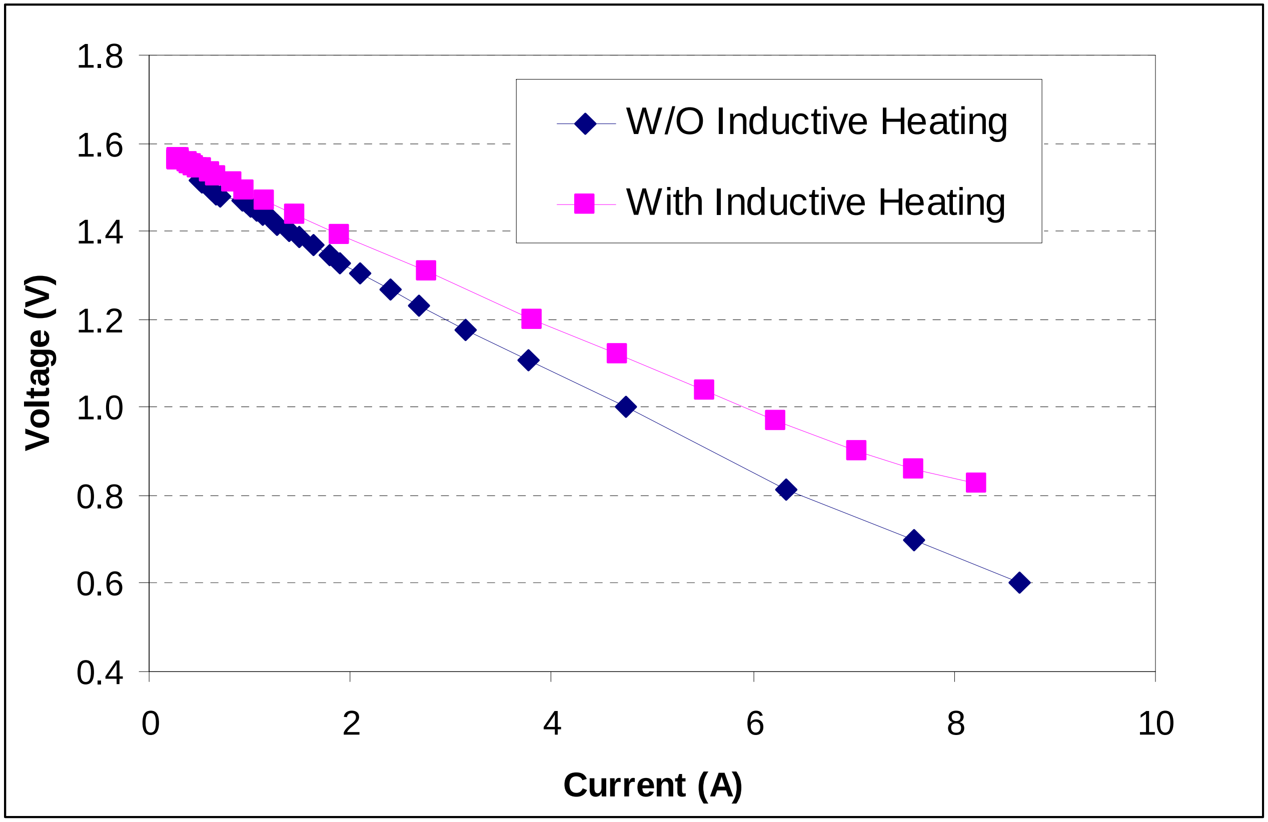
- Absorption and release is slow.
- ~ a few hours for a typical Ab/De-sorption cycle.
- Fast enough for stationary storage of renewable energy nevertheless.
- Can be expedited with innovative heating.
- For example inductive heating.

MgH_2: Fast release with induction Heating



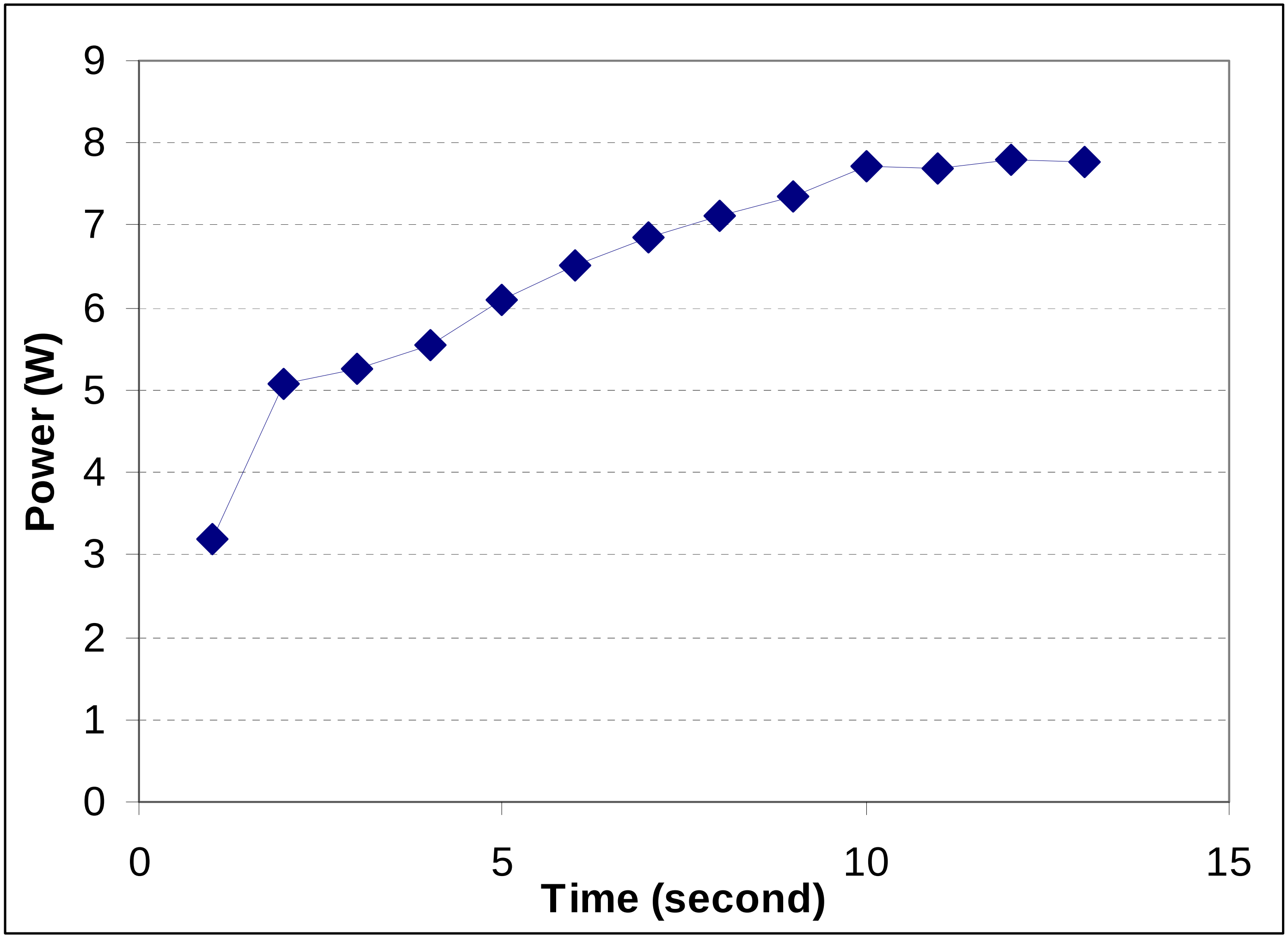


MgH_2: Fast release with induction heating



Fuel cell performance with and without induction heating

MgH_2: Fast release with induction heating



Fast fuel cell ramping with induction heating

Complex metal hydrides

The hydrogen bonding is more covalent or localized

- Examples: $Ca(BH_4)_2$, $Mg(BH_4)_2$, $LiNH_2$, $LiAlH_4$
- New development
- Many issues exist, like regeneration, volatiles, safeties

Final Year Downselection Path

$Mg(NH_3)_xB_{10}H_{10}$

$NaSc(BH_4)_4$ $Mg(B_3H_8)_2$ $Li_3AlH_6/2LiBH_4$ MgH_2/TiH_2 $(NH_4)_2B_{12}H_{12}$

$Li_2B_{12}H_{12}/2CaH_2$ AlB_4H_{11}

$LiBH_4/MgH_2$@ aero. $LiNH_2$

$Mg(BH_4)_2$@ aero

$Al/LiBH_4$ $MgB_{12}H_{12}$

$2LiNH_2/MgH_2$ $ANH_2/B(BH_4)_x$

$NaPB_2H_8$ $4LiBH_4/Mg_2NiH_4$ $Ti(BH_4)_3$

Materials examined in final year of the MHCoE

11 More Downselects
(Removing from Study)

$4LiBH_4/Mg_2NiH_4$	(low wt. %)
$Mg(B_3H_8)_2$	(too unstable)
$Li_2B_{12}H_{12}/2CaH_2$	(too high T_{des})
$Mg(NH_3)_xB_{10}H_{10}$	(NH_3 release)
$Mg(NH_3)_6B_{12}H_{12}$	(NH_3 release)

$CaB_{12}H_{12}/CaH_2$	(not reversible)
$Li_2B_{12}H_{12}/6MgH_2$	(too high T_{des})
$Ti(BH_4)_3$	(not reversible)
$Li_3AlH_6/2LiBH_4$	(too high T_{des})
$Li(NH_3)_xB_{12}H_{12}$	(NH_3 release)
$NaBP_2H_8$	(not reversible)

Physical/Chemical Sorption

- Basically utilize the relatively weak forces: Van Der Waals force, hydrogen bonding…
- Sometimes the sorption could also have a chemical nature.
- Examples: activated carbon, zeolite, MOF (metal organic framework), COF (covalent organic framework), nanotubes…

MOF

- **One of best known MOF 177:**

  $Zn_4O(BTB)_2$, where BTB^{3-} = 1,3,5-benzenetribenzoate

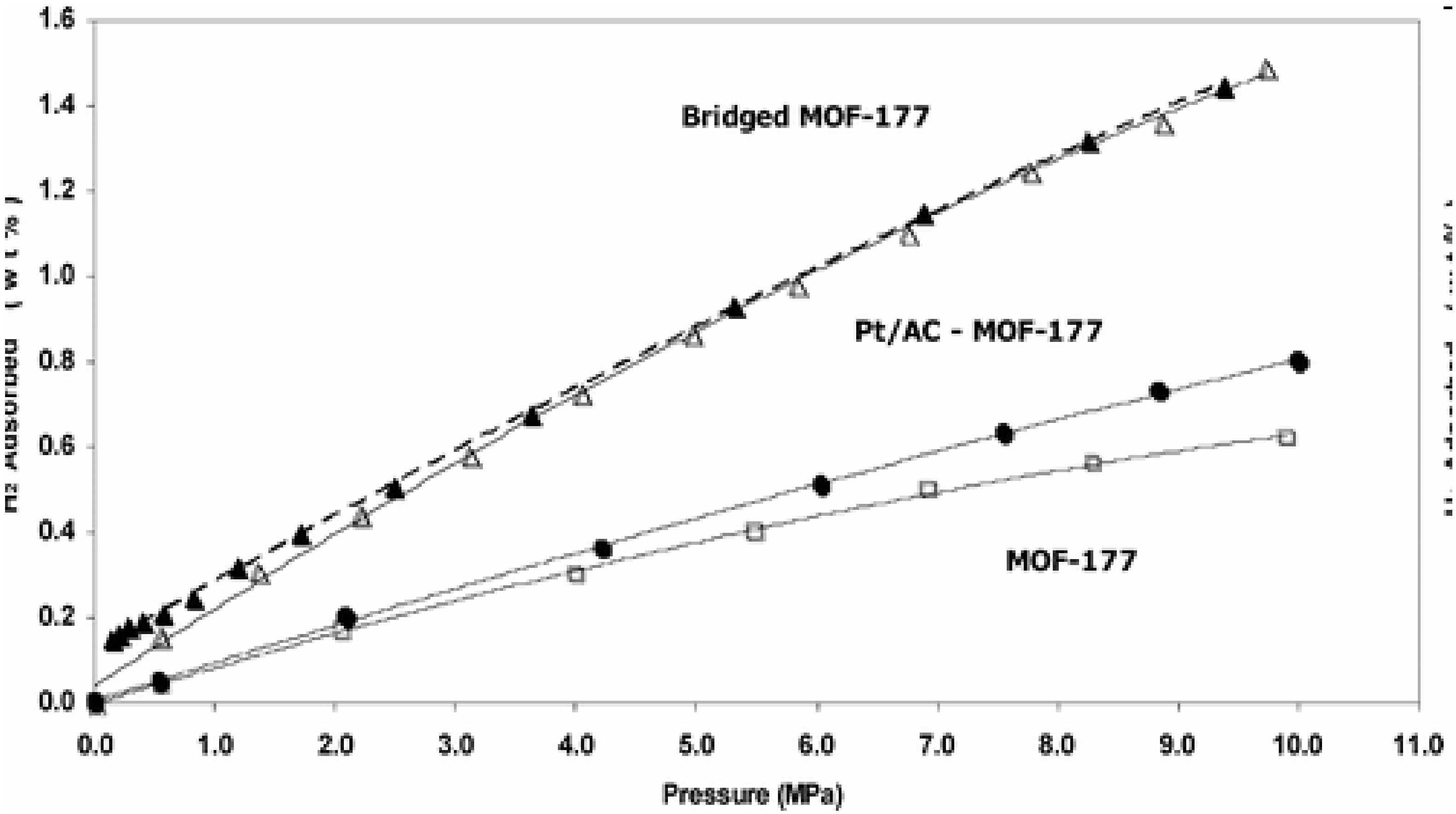
  Theoretical gravimetric density

  7.1 wt% at 77 K, 40 bar

  (not including dewar and pressure vessel)

  11.4 wt% at 77 K, 78 bar

MOF 177



Bridged MOF-177
Pt/AC - MOF-177
MOF-177
Pressure (MPa)
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0

Physical/Chemical Sorption

Some remarks

- MOF still not matching the AB_5 metal hydride in gravimetric density
- Generally poor volumetric density (puffy material)
- Cycling and cycle life?
- Good with cryogenic means