Thermodynamics Aspects of Hydrogen Storage in Metals

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Mech 6661

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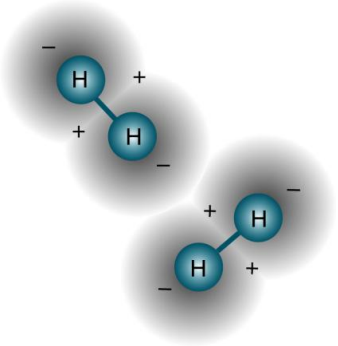
Outline

- Introduction
- Thermodynamics of H2 Fuel Cells
- Thermodynamics of H2 storage
- Concluding Remarks

1. Introduction

Introduction



A. Lulianelli, A. Basile, Catal. Sci. Technol., 2011

- Why Hydrogen Energy?
  1. Reduction in GHG emission
  2. Reduction of oil dependency
  3. Energy efficiency increase (conv. 20% → elec. 45%)

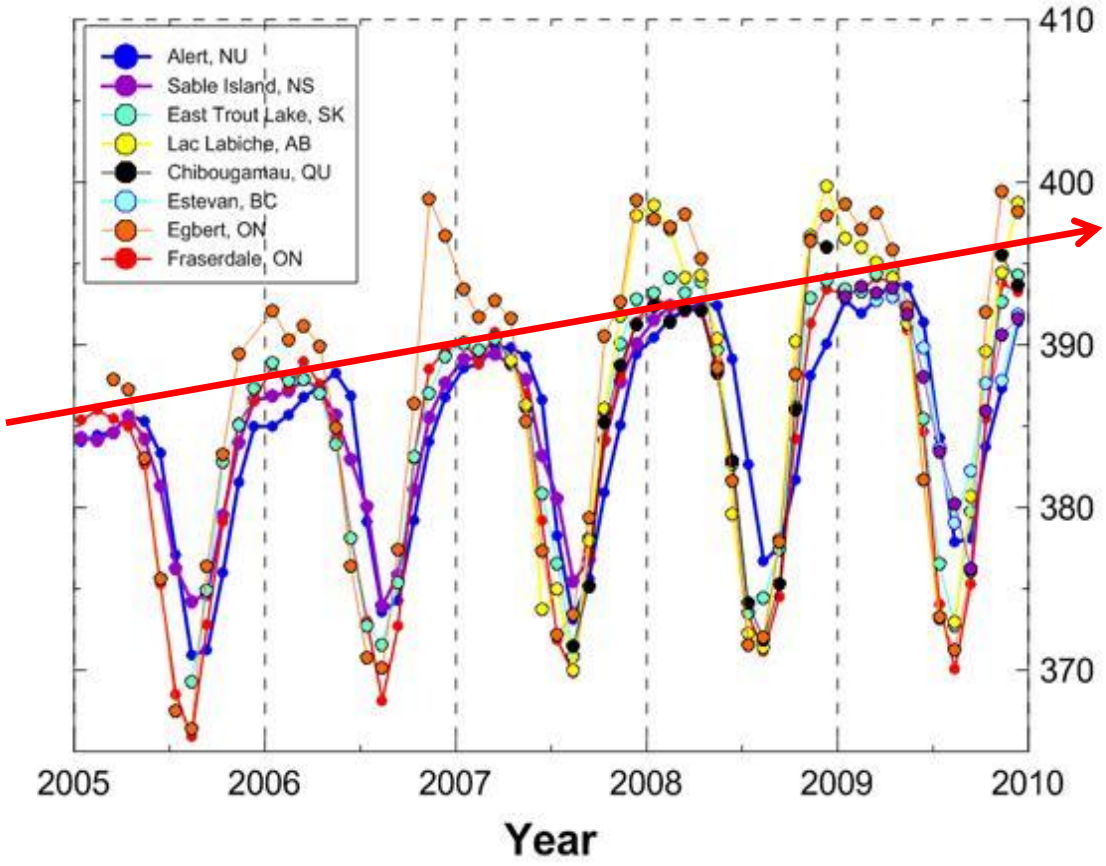
- What is Hydrogen Energy?
  - H2 is an Ultra High performance battery (Energy carrier)
  - **Hydrogen = Electrification**

- When?
  - 2015 →100 000 electric cars target in Europe

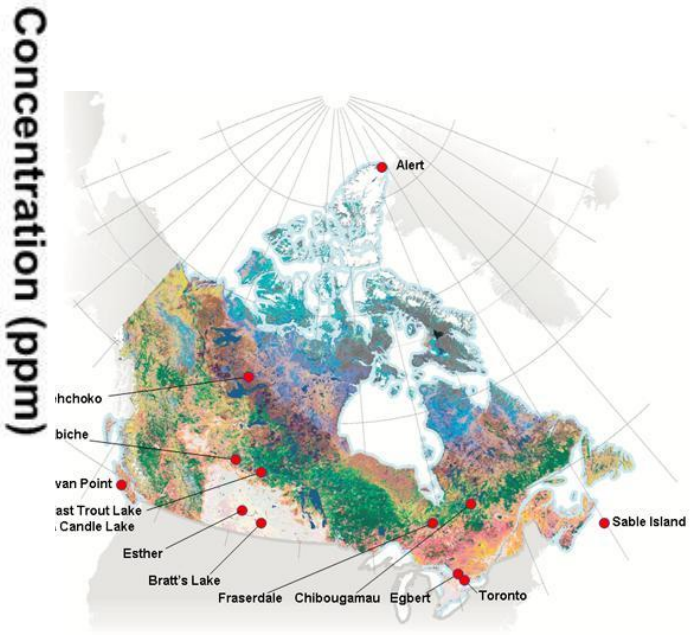
Palcan Energy, Canada

Canadian Interest in H_2

- 18,608,297 cars in 2005 Canada (620/1000) Natural Resources Canada 2011



Environment Canada, 2011



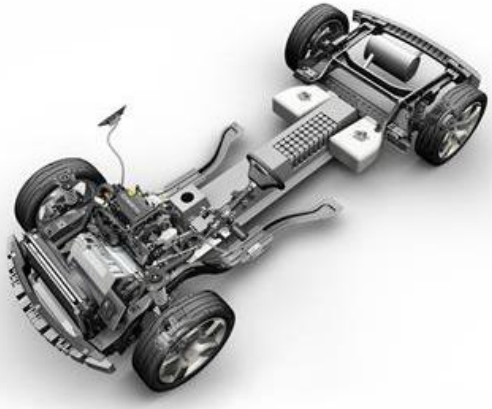
Environment Canada, 2011

Electric Vehicles Classification (EV)

- HEV: Hybrid Electric Vehicle

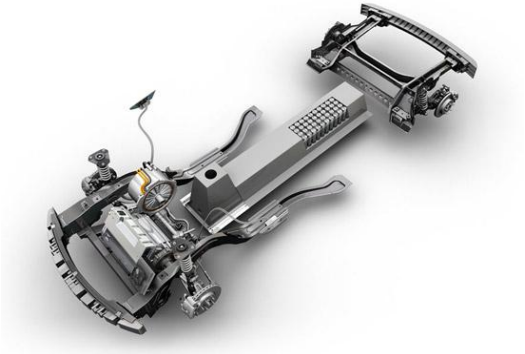
  Electric Motor + ICE + Battery

  3-50KW



- PHEV: Plug In Hybrid Electric Vehicle

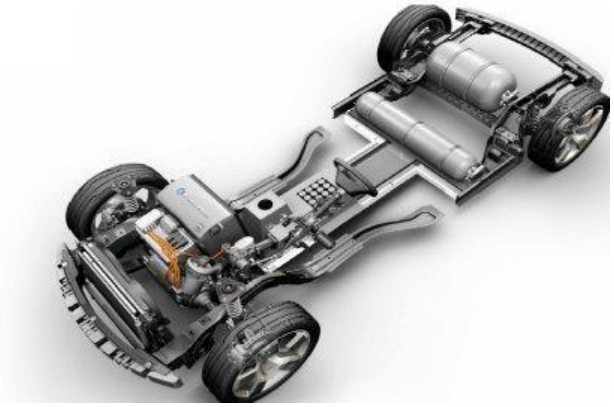
  Large Battery + Electric Motor 100+KW



- FCEV: Fuel Cell Electric Vehicle

H2 Tank + Fuel Cell + Small Battery

Electric Motor 75 KW

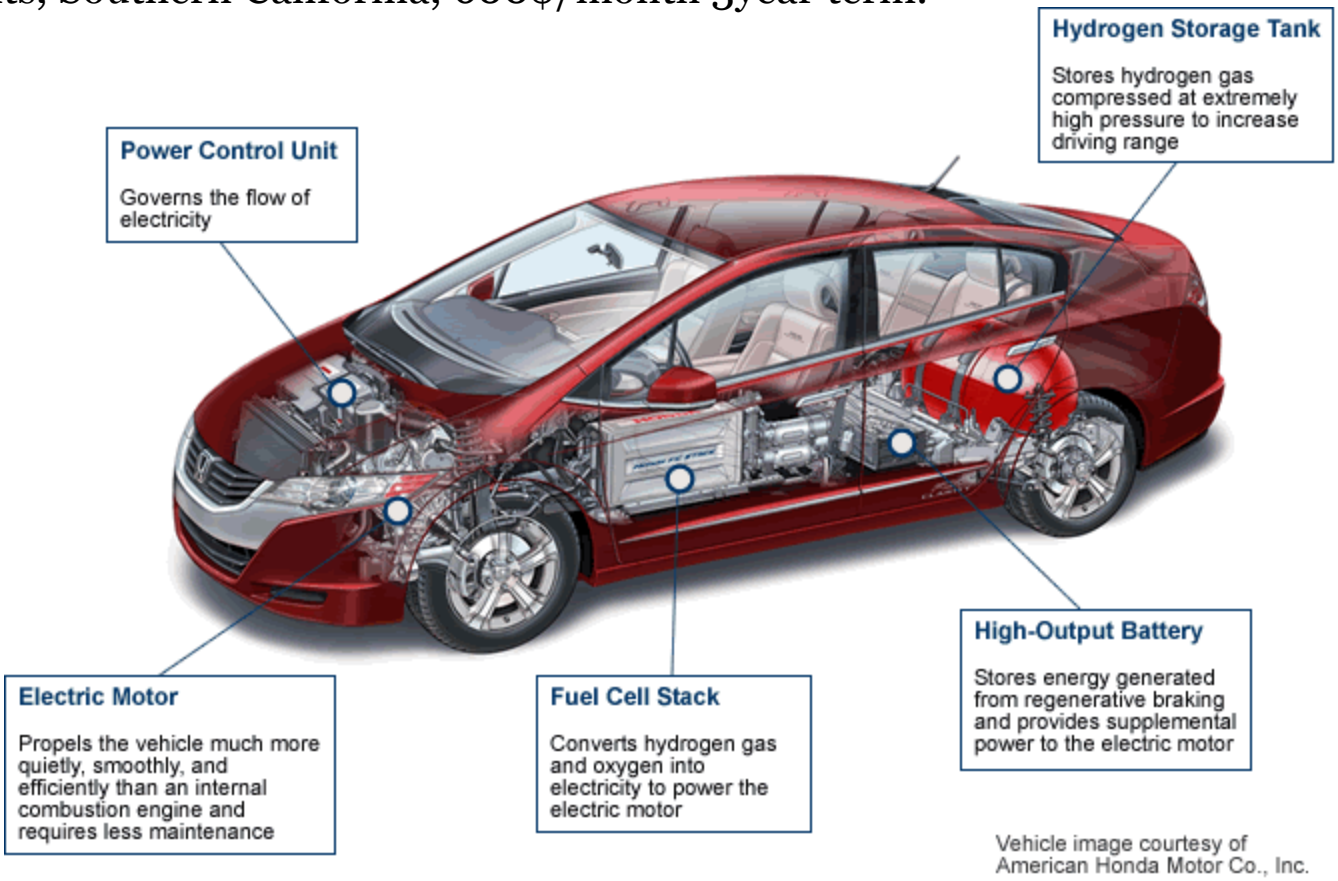


Images: SAE Presentation, Dr. James Gover, Kettering University

H_2 Powered Vehicles (FCEV)

- 2011 Honda FCX Clarity

200 units, Southern California, 600$/month 3year term.



http://automobiles.honda.com/fcx-clarity/

2.
Thermodynamics of Fuel Cells

Electrochemical Cell "Engine"

- Open System with Mass Flow, Work and Heat
  - Classical Thermodynamics crucial for design & control of the system.

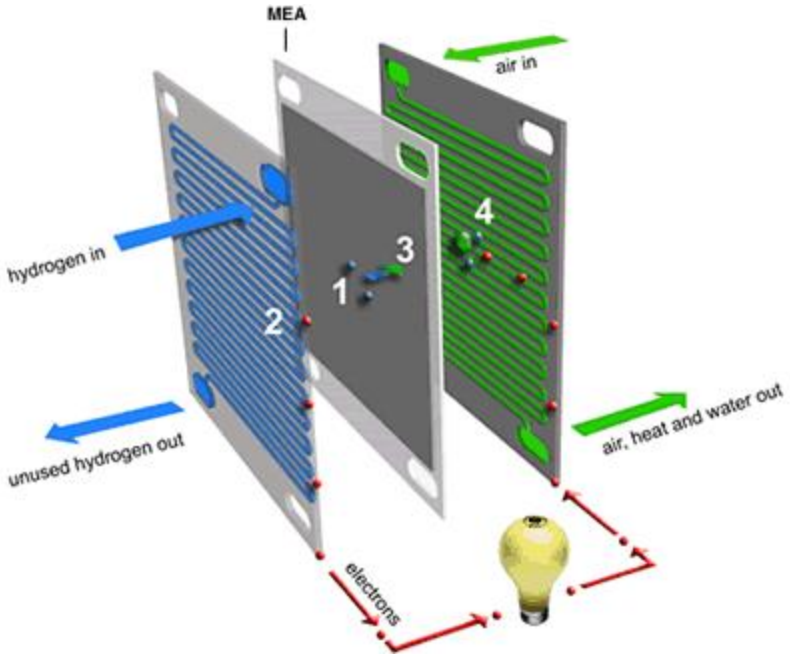
1st Law of Thermodynamics

$$\Delta U = Q - W$$

ΔU = Internal Energy

Q = Heat Added

W = Work Done



http://www.alternative-energy-news.info/technology/fuel-cells/

FactSage

Chemical reactions: Operating Conditions,
Material development, etc.

Fuel Cells Operation

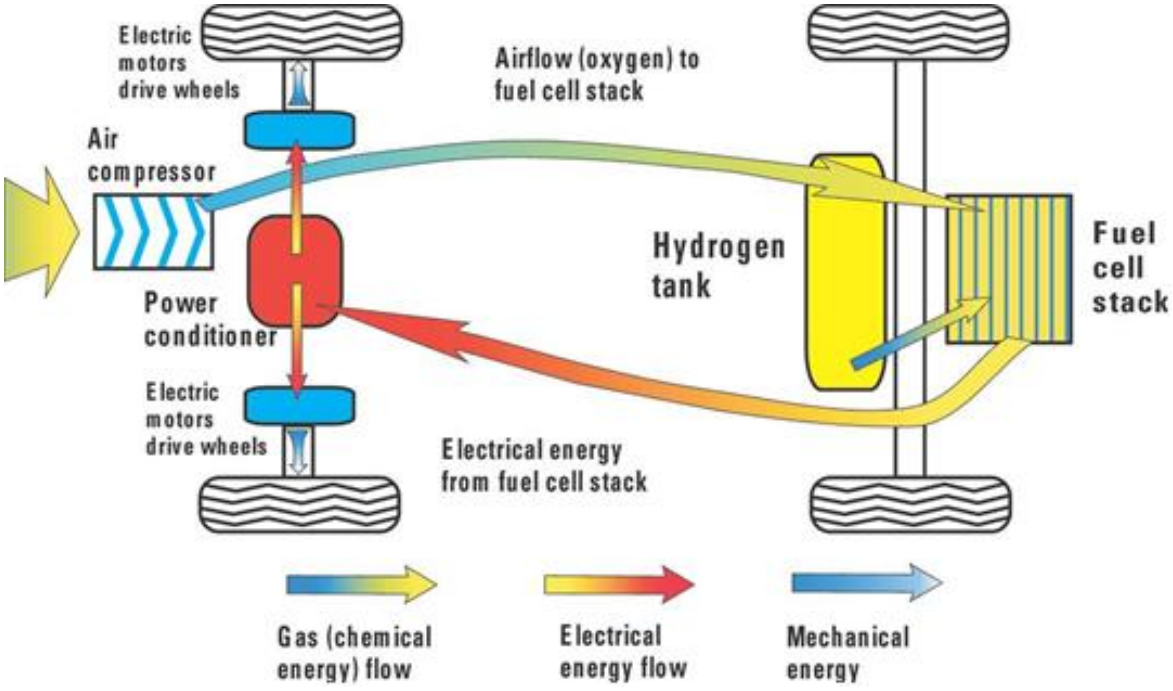
- At system level: Irreversible conversions

Chemical E. → Electrical E. → Mechanical E.

2nd Law of Thermodynamics

$$dS \geq \delta q/T$$

S = Entropy
δq = Heat Added
T = Temperature



Gerry Nolan, Silicon Chip, Issue 166, July 6 2002

FactSage

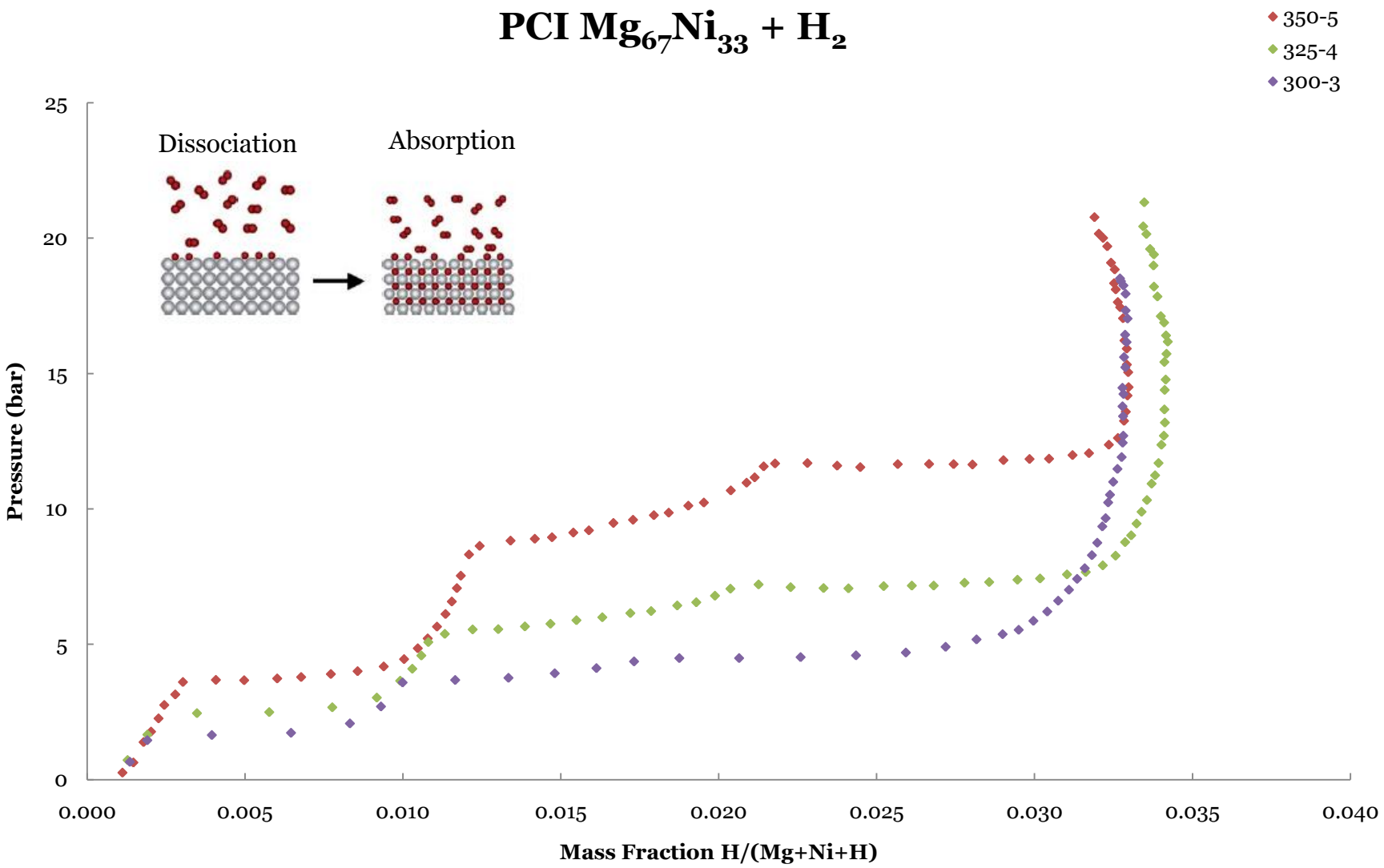
Operating Conditions,
Material development, etc.

3.
Thermodynamics of H_2 Storage

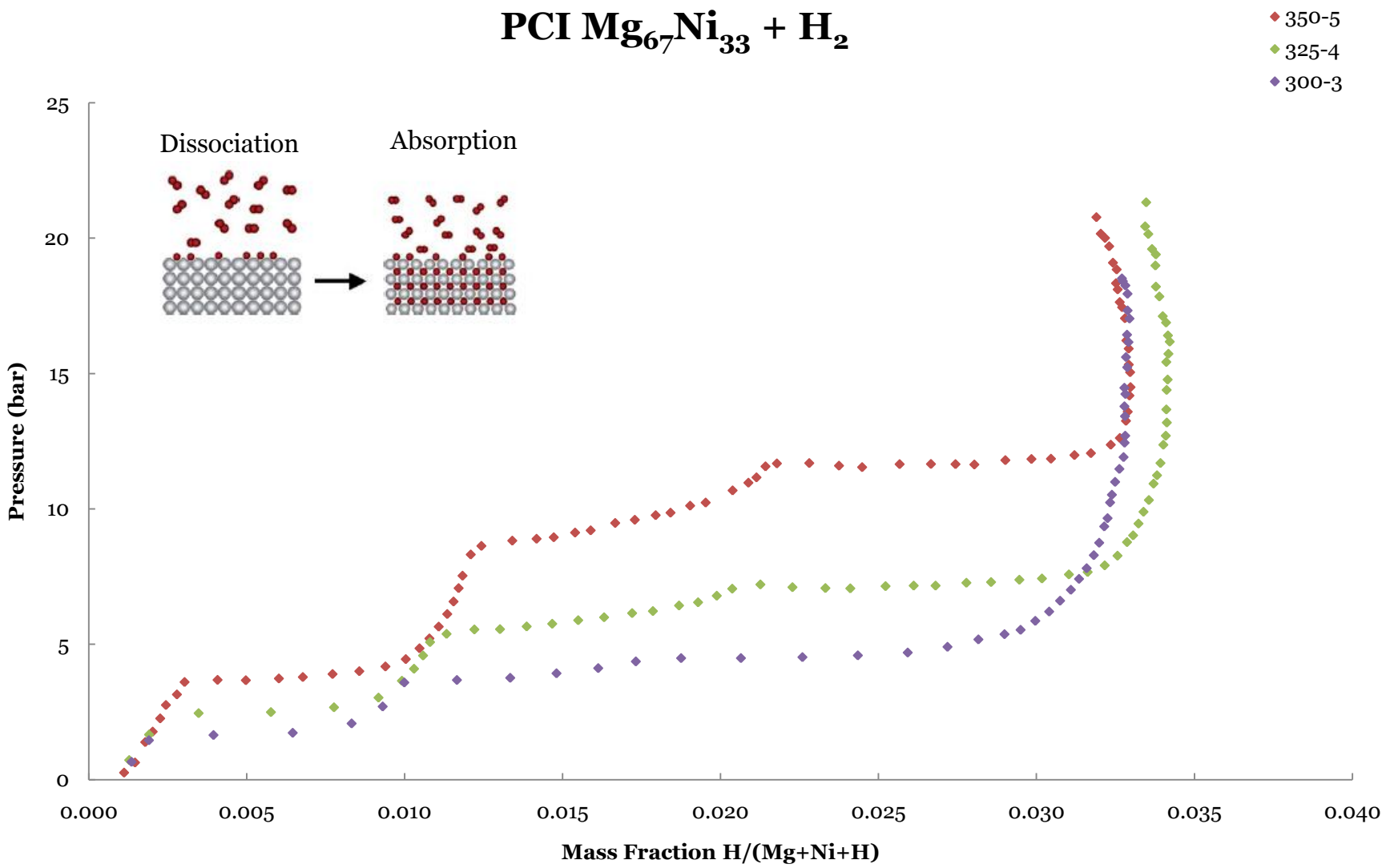
Thermodynamics of H_2 Storage

- Compressed Gas → Internal Energy Change
- Liquid H2 → Phase Change
- Adsorption → Weak Physical Bonding
- Metal/Complex Hydrides → Chemical Bonding
- Chemical Reactions → Product Generation

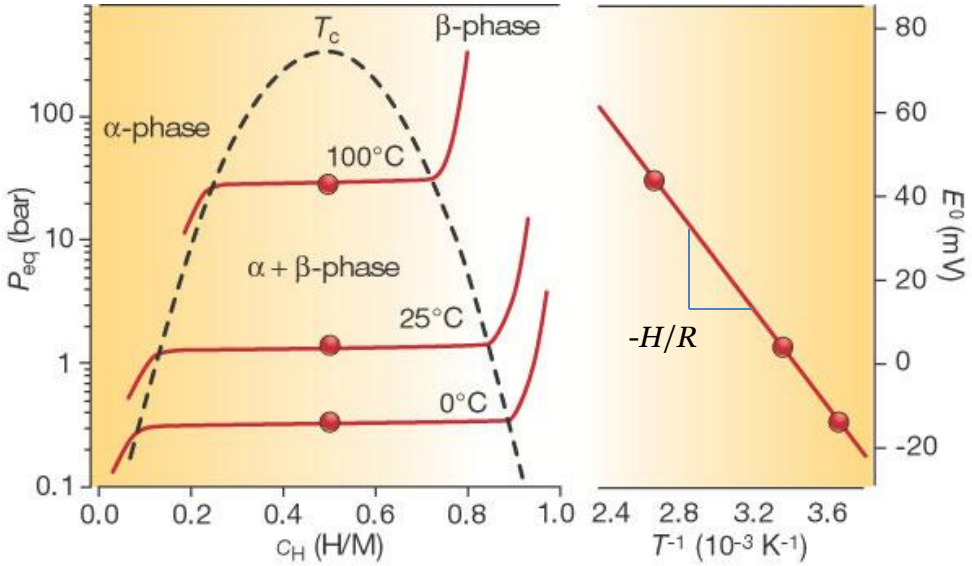
Metal hydrides Theory



Thermodynamic Modelling



Thermodynamics Analysis Tools

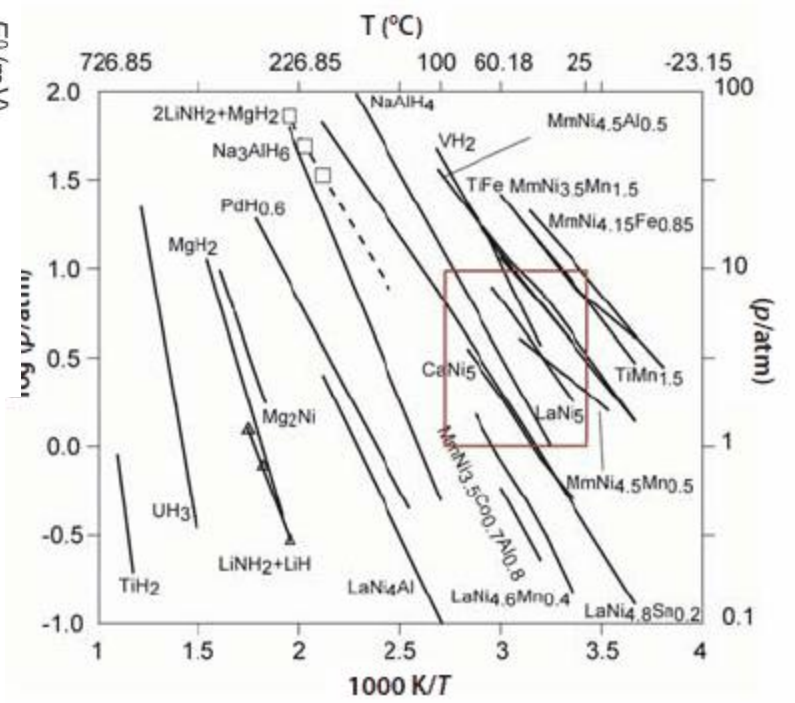


The Van't Hoff plot derived from the isotherms at various temperatures.

Nature 414, 353-358, 2001

The Van't Hoff equation

$$\ln(_{eq}/_{eq}{}^{o}) = (-H/R)(1/T) + S/R$$



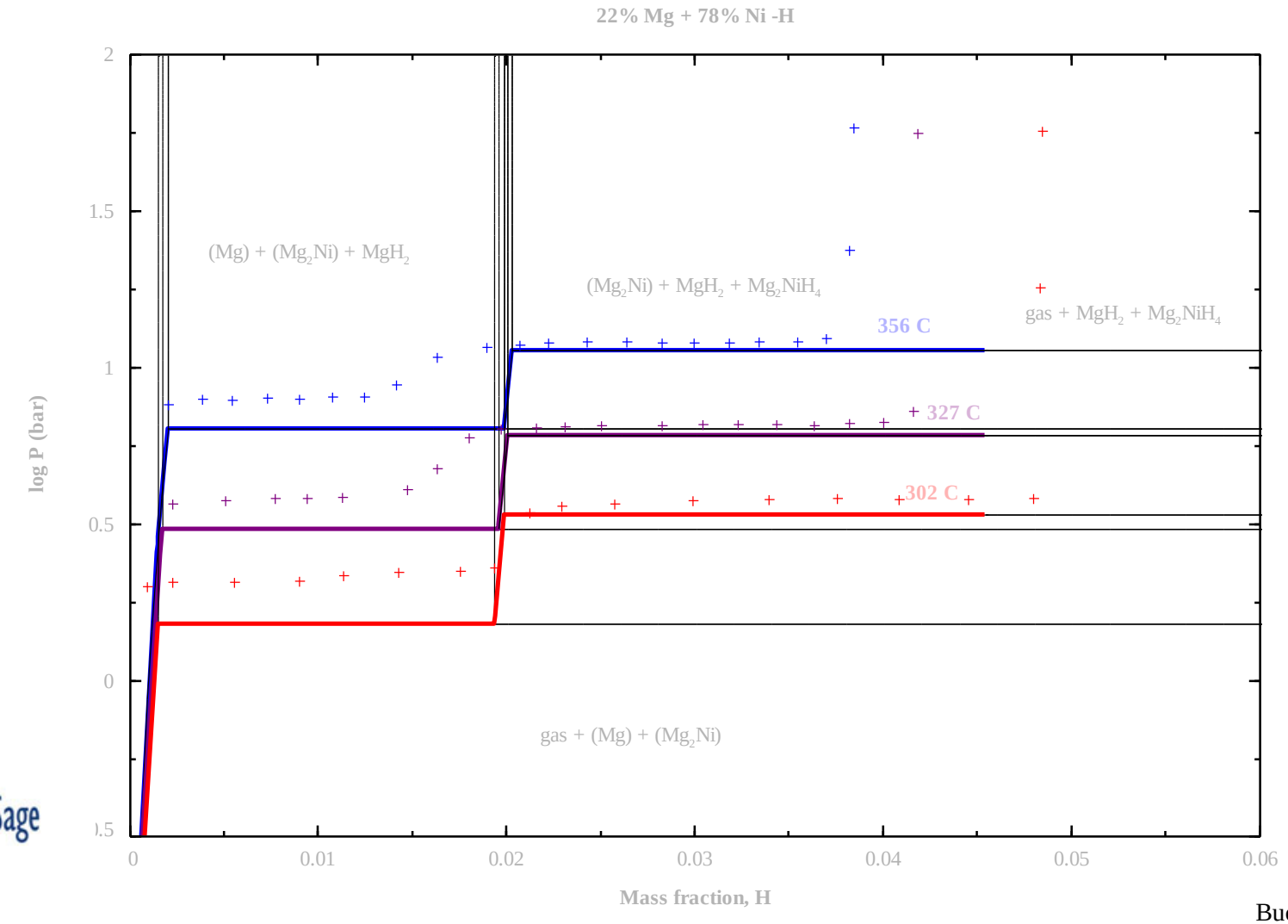
A compilation of the Van't Hoff plots of selected elemental, classical, and complex hydrides.

Material Matters, Volume 6, Article 2, 2011

Thermodynamic Modelling

- Why?
  - Experimental investigation time consuming
- Models:
  - Liquid → Quasi-Chemical
  - Solid Solution → Sublattice with random substitution
- Experiments provide:
  - $\Delta H_{hydride}$, Solubility range, etc.

Modelling vs Experimental data



Buchner ,1978

4.
Concluding Remarks

Concluding Remarks

- Classical & Statistical Thermodynamics essential for Hydrogen technologies .
- Thermodynamic Modelling with key experiment allows to faster investigation.
- Multidisciplinary investigations linked through thermodynamics laws.
- Renewable & Sustainable Energy?

? ¿ Questions ¿?

THANK YOU ☺