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Hydrogen supply and energy storage through the reaction of light hydrides: Technical assessment,

Thomas Laude

ABSTRACT

This report provides a technical assessment of different chemicals for a system that offers both hydrogen supply and energy storage, as needed for fuel cell applications. The technologies considered are the hydrogen release by the reaction of light-hydrides (ex: $\text{LiH} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{LiOH}$), and the energy filling by an efficient electrochemical recycling of the by-products. To identify the most promising candidate systems, we studied the thermo-chemical and physical data.

For the reactive release of H_2 , we considered the reaction of H_2O with strong reductors: LiH , Li , NaH , Na , NaBH_4 , MgH_2 , BeH_2 and AlH_3 . All hydrides showed potential for an excellent storage density, competitive to that of gasoline, and acceptable energy efficiency on release (in the order of 70%). The metals (Li and Na) had lower potential for both density and efficiency (by about a factor two). We also considered replacing H_2O with NH_3 in the release reaction. $\text{LiH} + \text{NH}_3$ reaction may provide excellent release efficiency thanks to endothermicity and to good storage density. However, this system suffers of NH_3 storage requirements and probably of low reactivity.

For an energy efficient recycling of the hydroxide, we considered melted salt electrolysis. Only LiOH and NaOH may be recycled in this way because other hydroxides do not have a stable liquid phase. We conclude that for a recycled system, LiH is favoured for its high storage density, but NaH is potentially cheaper to cycle thanks to better energy efficiency. We propose a simple design for the supply system that could allow both releasing and filling in the same closed box, with heat recycling on filling. The system is preferably filled by hydrogen and electricity, but may also be filled by electricity only.

We also led a cost comparison. We conclude that, for chemically-cycled storage, lithium has an over-cost of +22% compared to sodium due to higher heat loss on release, provided that lithium could be cycled over 100 times. For storage systems without chemical recycling, the most economical candidates are AlH_3 and NaH , for which the metal hydride cost is estimated approximately 7 euro per kg of H_2 stored. For large scale usage, a chemical recycling will be necessary.

Based upon the review of the different systems, the LiH system with electrolysis as a regeneration step appears to be the most promising system, in particular for fuel cell applications where high-density and reasonable energy cost is needed, like long range distribution or automotive. The system has been very lightly studied in the literature, and only using a different regeneration step than the one presented here. We also conclude that a similar system based on sodium is a viable candidate for some applications thanks to its lower energy cost, and although it offers lower energy density.

As a first step, we propose to evaluate the feasibility of the LiOH and NaOH electrolyses and to measure the associated energetical and chemical efficiencies experimentally. Based on the

success of this first step, we could then evaluate the total cyclability of the reactions, and finally develop a prototype system.

In a more remote future, we expect additional developments of the technology. The exothermal release could be coupled with an endothermic release, to improve the overall energy efficiency. The system could be coupled to a fuel cell to offer an electricity-to-electricity storage solution. Energy density could be higher by several orders compared to existing electrical storage devices, and at acceptable energy efficiency (say 30%). Finally, similar $\text{AlH}_3 + \text{H}_2\text{O}$, and $\text{NaH} + \text{H}_2\text{O}$ reactions could be used in a non-chemically-recycled hydrogen supply, where metals would be discarded after use. This would provide a simple and high density solution in some niche applications where higher energy cost can be afforded.

1. Introduction

One of the major technical challenges to be overcome for the large spread utilization of hydrogen fuel cells for applications such as transportation or general consumer use is to develop efficient and safe storage technology. High pressure hydrogen cylinders (up to 700 bar) are under development but still suffer from a relatively low energy storage density. Liquid hydrogen systems must consider the boil-off from both a safety and an efficiency perspective. Hydrogen storage systems based on the decomposition of metal hydrides have a mass storage limited to about 2%mass (mass of hydrogen to metal).

An alternative more recently studied is the energy storage in light hydrides and the hydrogen release from their reaction with water. (It should be noticed that reactive chemical supply is different from direct storage of hydrogen, in that it enables storing the energy from non-hydrogen sources, in particular other chemicals, electricity or heat, and to generate hydrogen only in the final release step. Hence, energy storage and hydrogen supply are separated functions.) This offers a high density of energy storage from both a mass and volume perspectives. Such systems have proven feasible, and in particular with sodium borohydride (NaBH_4), but the hydrides have also proven expensive to produce. For this reason, in this report, we mostly consider light hydrides that have the potential to be recycled in an energy efficient way, typically by electrolysis, or at least that are cheap to produce.

The qualities of a hydrogen supply and energy storage system are firstly storage density and cost. Energy density should be high, both for mass and volume. Cost should be low, considering both the materials used for the storage, but also the efficiency of the system when filling, releasing and over storage time. Then, energy input (hydrogen, electricity, heat or chemicals) should be cheap. Preferably, all chemicals produced apart from hydrogen should be recyclable, to reduce chemical cost (and waste). Finally, the system itself should be inexpensive while providing means for acceptable safety level. For a recyclable chemical storage, as considered here, the global cost is firstly determined by the efficiency factors on filling and on release.

In addition to these factors, the environmental impact should be low. The storage should be easy to use, if possible avoiding extensive external re-treatments. The hydrogen produced should be sufficiently pure for the fuel cell and with reliable flow.

The following report focuses on a hydrogen supply system for a fuel cell using reactive release of type $AH_x + BH_y \rightarrow H_2 + ABH_z$, where A and B are light elements (period 2 and 3 of element table) and where ABH_z can be recycled back to the reactants. Such reaction may be exothermic or endothermic. This is different from more common storage with decomposition release $AH_x \rightarrow x/2 H_2 + A$, which is always endothermic.

Obviously, water is a preferable reactant because it can be recycled from the fuel cell. Water is also preferable because it does not involve additional elements than those in the fuel cell. Therefore, most release reactions considered here are of type $H_2O + BH_y \rightarrow H_2 + B(OH)_z$. However, we also consider non- H_2O reactions, in particular NH_3 based reactions.

The front running release reaction studied here is $LiH + H_2O \rightarrow H_2 + LiOH$. Other reactions can be considered as a variation from this one:

- Li instead of LiH
- NaH, Na and $NaBH_4$ instead of LiH
- MgH_2 , BeH_2 instead of LiH
- AlH_3 instead of LiH
- NH_3 instead of H_2O

For each of these chemical families, we considered the thermodynamics of the different steps in the cycle, e.g. the release (H_2 release by reaction of the metal hydride with either H_2O or NH_3), and the filling (re-generation of the hydride from the by-product of the release step). Then the ideal energy efficiency was estimated for the different systems considering heat (enthalpy) losses. (For this report, it may be useful to memorize the enthalpy of combustion of hydrogen $H_2 + 1/2O_2 \rightarrow H_2O_{liq}$: 286 kJ/mol at 20C.)

Then, we estimated the ideal storage density, not considering the mass of water when it can be recycled from the fuel cell. [For simplification we considered that one H_2O molecule can be recycled for one H_2 molecule stored. A more realistic figure is probably around 90-95% (see annex).] Also, we considered no voids in powders (chemical volume as liquid) or system volume, so that volumetric density obtained should only be seen as an ideal maximal value. Examples are given for a 7kg H_2 supply system which corresponds to a car application (7kg hydrogen corresponds to ~ 57 liters of gasoline, assuming that a hydrogen fuel cell with an electric motor enables twice the energy efficiency of a gasoline motor) but is not limited to that dimension.

Finally, we considered the technical feasibility of the systems, taking in account the

requirements of the materials at temperatures and other conditions along the cycle.

2. How we select the reactions

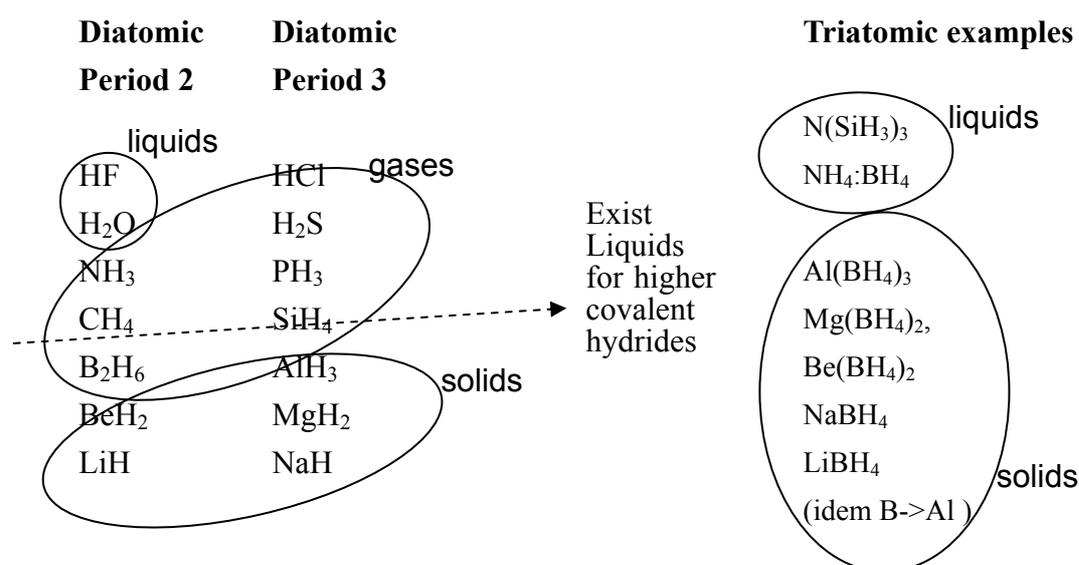
2.1. Available reactions

Apart from obvious H_2O , the choice of reactants is limited once we consider the following requirements:

- Mass ratio of released H_2 to carried compounds should be high, at start and at end of the reaction
- The number of elements involved should be limited for recycling (monoatomic and diatomic compounds are preferable to triatomic compounds).
- Both reactants should be stored as a liquid or a solid (preferably at 1 bar, and preferably within the reactor), for high volumetric density
- Reactants should not be both solids (preferably liquids) for reactivity and handling considerations
- Final product should not cover reactants and impede reaction
- Final product should be recyclable in energy efficient way
- Reactant cost should be low

To have a simple triatomic chemistry, we consider reaction between a hydride (AH_x) and another compound that do not bring more than 1 additional element (B) to the system (a pure compound or another hydride). Gas being cumbersome for storage, we favour a reaction liquid + solid, or liquid + liquid. So, the first step is to select a liquid hydride (there is no liquid among pure light elements).

Available Hydrides

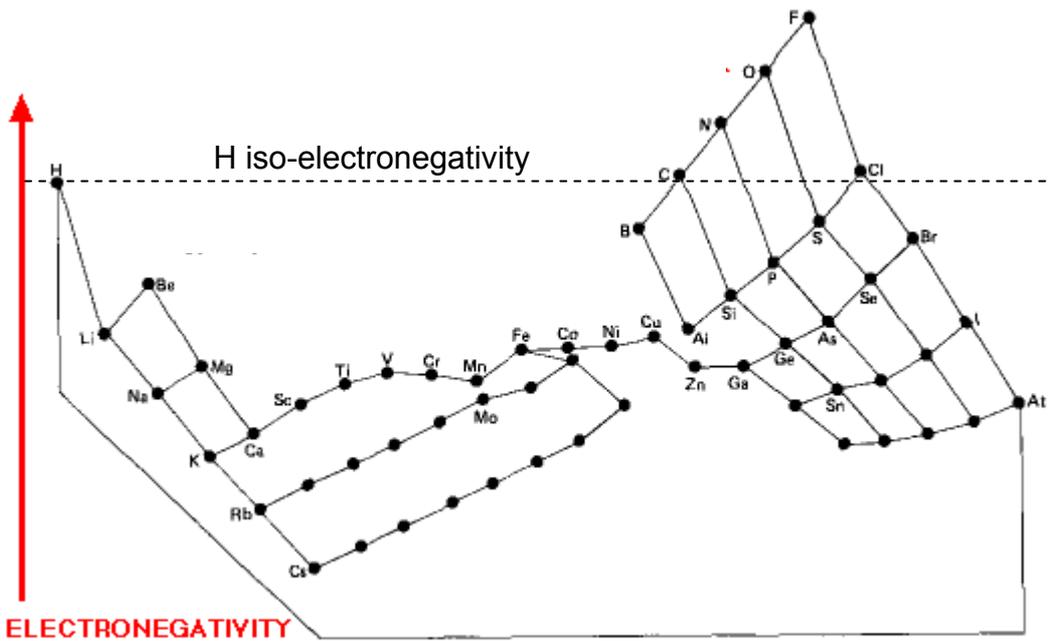


The choice for liquid hydrides is limited:

- HF is excluded for safety.

- Hydrocarbons suffer of isoelectronegativity of H and C (ex: Burning leads to both oxide). The reaction of $H_2O + \text{hydrocarbon} \rightarrow H_2 + CO_2$ (reforming) is possible but endothermic and produces CO_2 .
- Higher B and Si hydrides are interesting but fall out of the scope of this report, for their complexity.

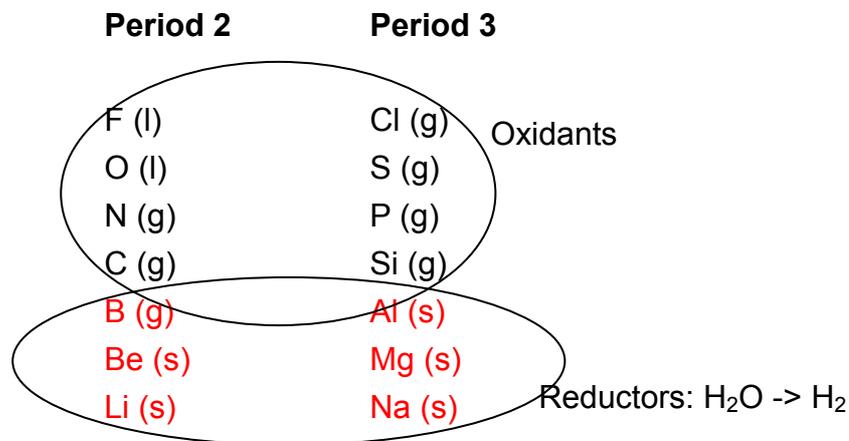
For these reasons, we mostly consider the reactions of H_2O with solid (and electropositive) elements or their diatomic hydrides. But we will also consider one reaction with a triatomic hydride ($NaBH_4 + H_2O$), and two gas + solid reactions ($2Li + 2/3NH_3(g) \rightarrow H_2 + 2/3Li_3N$ and $LiH + 1/3NH_3(g) \rightarrow H_2 + 1/3Li_3N$).



Electronegativity of the elements, as obtained from <http://users.rcn.com/jkimball.ma.ultranet/BiologyPages/E/Electronegativity.html>

2.2. Release reactions with water

2.2.1. Reactions of elements with water:

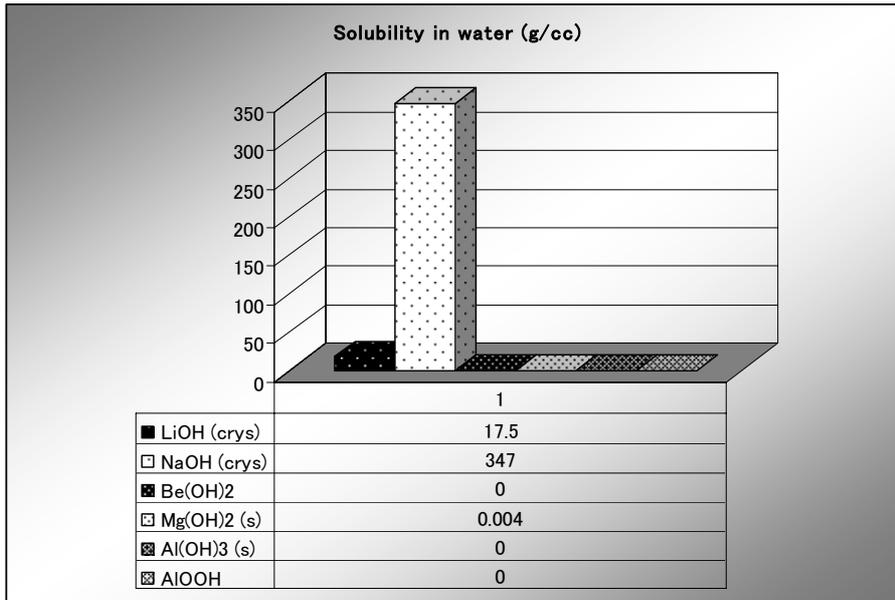


Only, the strong reductor elements are available for water reduction, with H₂ release:

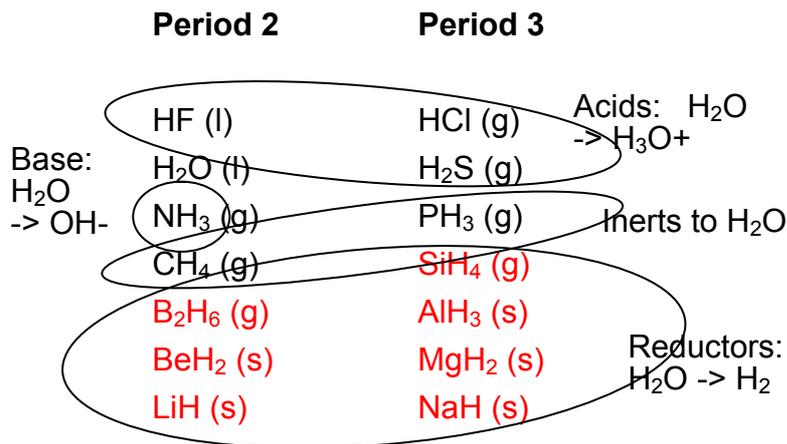
- $2\text{Li} + 2\text{H}_2\text{O} \rightarrow \text{H}_2 + 2\text{LiOH}$ ($\Delta G = -404\text{kJ/mol}$)
- $2\text{Na} + 2\text{H}_2\text{O} \rightarrow \text{H}_2 + 2\text{NaOH}$ ($\Delta G = -285\text{kJ/mol}$)
- $\text{Mg} + 2\text{H}_2\text{O} \rightarrow \text{H}_2 + \text{Mg(OH)}_2$ ($\Delta G = -359\text{kJ/mol}$)
- $\text{Be} + 2\text{H}_2\text{O} \rightarrow \text{H}_2 + \text{Be(OH)}_2$ ($\Delta G = -341\text{kJ/mol}$)
- $2/3\text{Al} + 2\text{H}_2\text{O} \rightarrow \text{H}_2 + 2/3\text{Al(OH)}_3$ (ΔG no data)
- $2/3\text{B} + 2\text{H}_2\text{O} \rightarrow \text{H}_2 + 2/3\text{B(OH)}_3$ (ΔG no data)

Note: All reaction involve simple red/ox reactions of type $2/nM + 2H^+ \rightarrow H_2 + 2/nM^{n+}$ (respective electrochemical potential of 3.04, 2.71, 2.37, 1.85, 1.662, 0.870 V, for Li, Na, Mg, Be, Al, B).

Although Li to Be reactions are thermodynamically viable, only Li and Na reactions have been reported experimentally. The reason is probably the formation of an insoluble hydroxide layer (and oxide if exposed to air) on the metal that inhibits the reaction for all elements except Na and Li (see hydroxide solubility graph below).



2.2.2. Reactions of diatomic hydrides with water



Again, the strong reductor hydrides are available for water reduction, with H₂ release. Note that H₂ is released from the water and not from the hydride. The resulting hydroxide may decompose to the oxide if unstable. This is the case at ambient for silicon (Si(OH)₄ → SiO₂ + 2 H₂O).

- ◆ LiH + H₂O → H₂ + LiOH (ΔG = -133kJ/mol)
- ◆ NaH + H₂O → H₂ + NaOH (ΔG = -109kJ/mol)
- ◆ 1/2Mg H₂ + H₂O → H₂ + 1/2Mg(OH)₂ (ΔG = -161kJ/mol)
- ◆ 1/2Be H₂ + H₂O → H₂ + 1/2Be(OH)₂ (ΔG = -149kJ/mol)
- ◆ 1/3AlH₃ + H₂O → H₂ + 1/3Al(OH)₃ (ΔG no data)
- ◆ 1/6B₂H₆ + H₂O → H₂ + 1/3B(OH)₃ (ΔG no data)
- ◆ 1/4SiH₄ + 1/2 H₂O → H₂ + 1/4SiO₂ (ΔG no data)

Note: Again, these reactions involve a simple red/ox reactions, but of type: H⁻ + H⁺ → H₂.

In this case, all above reactions are reported experimentally, although SiH_4 one is reported slow. As in the previous case, solid hydrides (all except for B_2H_6 and SiH_4) reaction speed probably depends on solubility of the hydroxide in water.

2.3. Recycling the hydroxide by melted salt electrolysis

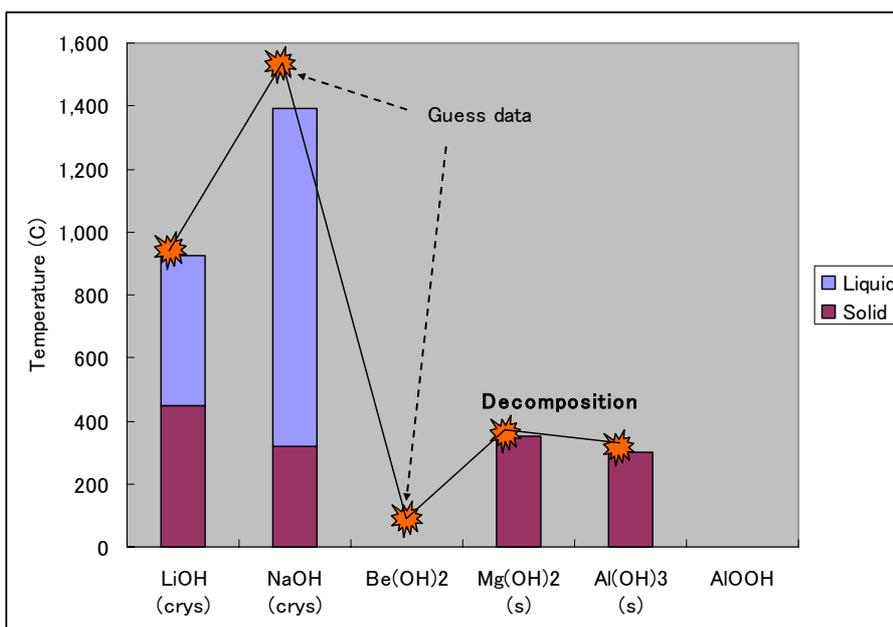
To recycle the hydroxide obtained after the hydrogen release reaction, melted salt electrolysis is considered as an energy efficient process. As the electrolysis reaction creates molecules and breaks bonds, the entropy of the reaction system increases and may be endothermic in nature. As a result, the thermal efficiency of the electrolysis reaction may be high. Endothermicity reduces heat losses from Joule effect, hence increase energy efficiency. The portion of heat absorbed to total electrical input increases with temperature. (This principle is well known for hot water electrolysis for instance.)

Exemple: electrolysis of melted LiOH:

Half reactions: $\text{Li}^+ + e^- \rightarrow \text{Li}$ and $\text{OH}^- + e^- \rightarrow 1/2 \text{H}_2\text{O}_{\text{gas}} + 1/4 \text{O}_2$

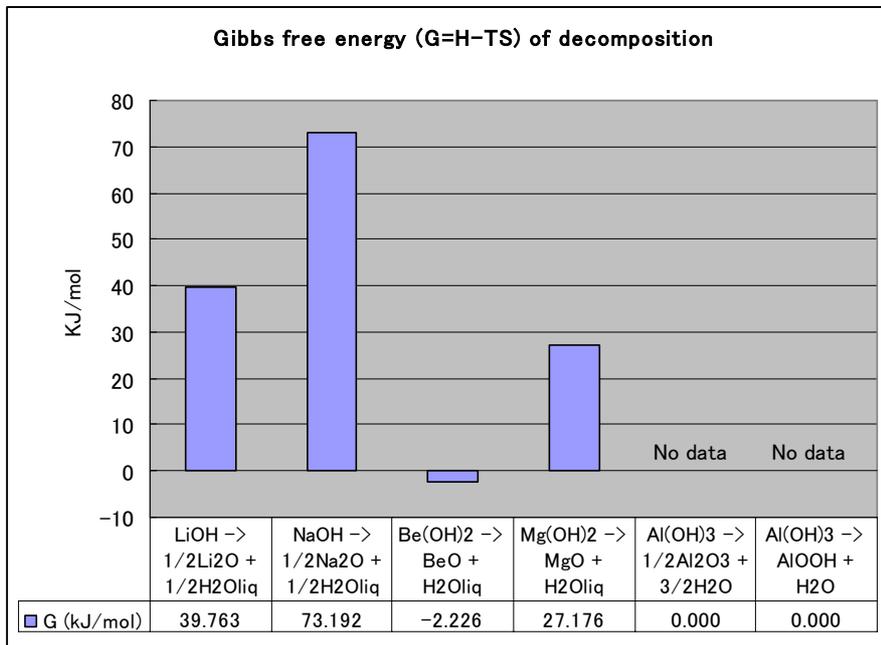
Global reaction: $\text{LiOH} \rightarrow \text{Li} + 1/2 \text{H}_2\text{O}_{\text{gas}} + 1/4 \text{O}_2$ (Enthalpy at room T: $\sim +366 \text{ kJ/mol}$)

For such electrolysis, high temperature is necessary both for energy efficiency and to melt the hydroxide. However, as the temperature rises, the hydroxide tends to decompose to the oxide releasing water. Oxides have a very high melting point, which makes them impractical for melted salt electrolysis. As a result, and as shown in the graph below, only Na and Li may be compatible with an electrolysis of the hydroxide. NaOH is liquid in the range 318-1390C. LiOH is liquid in the range 450-924C.



Note: for NaOH and Be(OH)₂, there is no data for decomposition temperature. However for NaOH,

the stability is known up to the boiling temperature, and for $\text{Be}(\text{OH})_2$, the stability can be expected very low as the free energy for decomposition reaction is already negative in standard conditions (graph below).



Note: G of different reactions is not strictly comparable, but the reactions being similar, it gives a hint of the stability/decomposition point

Finally, it should be understood that the electrolysis of NaOH and of LiOH and their efficiencies are still to be confirmed experimentally. Today, the literature on NaOH electrolysis is scarce, and the literature on LiOH electrolysis is almost inexistent. Hopefully, this is because such processes had no commercial interest up to now.

Note 1: recycling the hydroxide by thermo- reduction?:

Safe hydrogen LLC reported the following reaction for LiOH (from 1100C with CO removal):

$\text{LiOH} + \text{C} \rightarrow \text{Li} + \text{CO} + 1/2 \text{H}_2$ [This probably involves a decomposition step: $2\text{LiOH} \rightarrow \text{Li}_2\text{O} + \text{H}_2\text{O}$] Additional hydrogen is collected from $\text{CO} + \text{H}_2\text{Ogas} \rightarrow \text{CO}_2 + \text{H}_2$ reaction

This seems unpractical because:

- Temperature is high
- The reaction burns C to produce CO_2
- Feasibility is uncertain
- The system is complex
- The reaction produces more H_2 that it can later store

(PowerBall Technologies LLC reported a similar process for NaOH with $\text{NaOH} + \text{CH}_4$ reaction)

Note 2: Recycling the hydroxide by aqueous electrolysis?

LiOH and NaOH are soluble in water (dissolution enthalpy of -14 kJ/mol for LiOH). However aqueous electrolysis is not possible because reduced metal would react with water to give H_2 . The

global reaction would be an electrolysis of water, with heat losses.

3. Li/O/H based systems

3.1. Generalities

Stable compounds of Li, O and H: Li, LiOH, Li₂O, (Li₂O₂), O₂, H₂O, H₂

Li melting (C)	180
LiH melting (C)	689
LiOH melting (C)	450
LiOH decomposition (C)	924

A closed system with only 3 atoms (Li/O/H) involves a limited number of compounds, and hence is expected to cause few side reactions. This is important for hydrogen purity and for cyclability. While not tested yet, LiOH is expected to be cyclable because it is stable to the oxide. Also, although LiH can reduce only one H₂O molecule, Li is very light, so LiH provides a reasonably good storage density. Finally, the reactivity on H₂ release is expected sufficient because of the high solubility of LiOH and because of the electropositivity of Li.

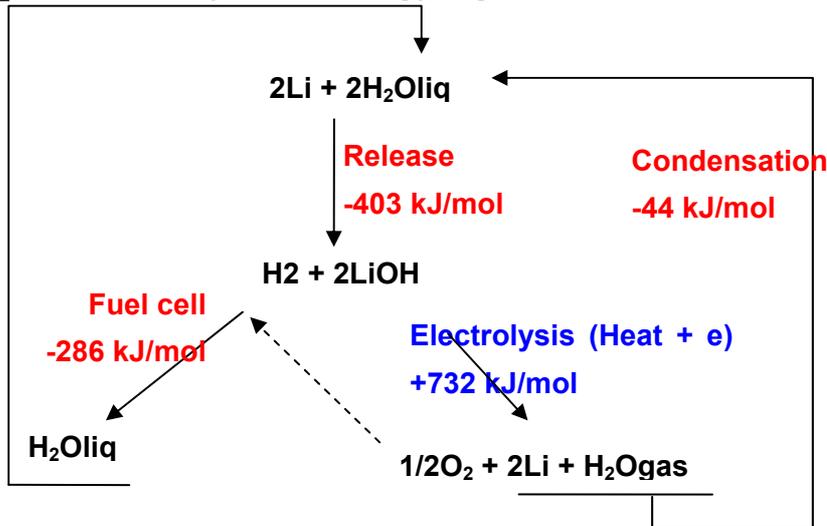
However, lithium has drawbacks too. In particular, LiOH is sensitive to atmospheric CO₂ to forms lithium carbonate impurities. Also Li and LiH are sensitive to atmospheric moisture and to oxygen. This may cause energy losses on storage. For these reasons, a closed and well sealed system is preferred to a fuel-like commodity.

We will see that a Li/O/H based system may be refilled directly, either by electricity and heat (Li storage), or more efficiently by electricity, heat and hydrogen (LiH storage)

Known actors on similar reactions: Safe hydrogen LLC [LiH slurry (mix with oil) storage, LiH+H₂O release, reduction recycling with C at 1100C]

3.2. Reaction pathway

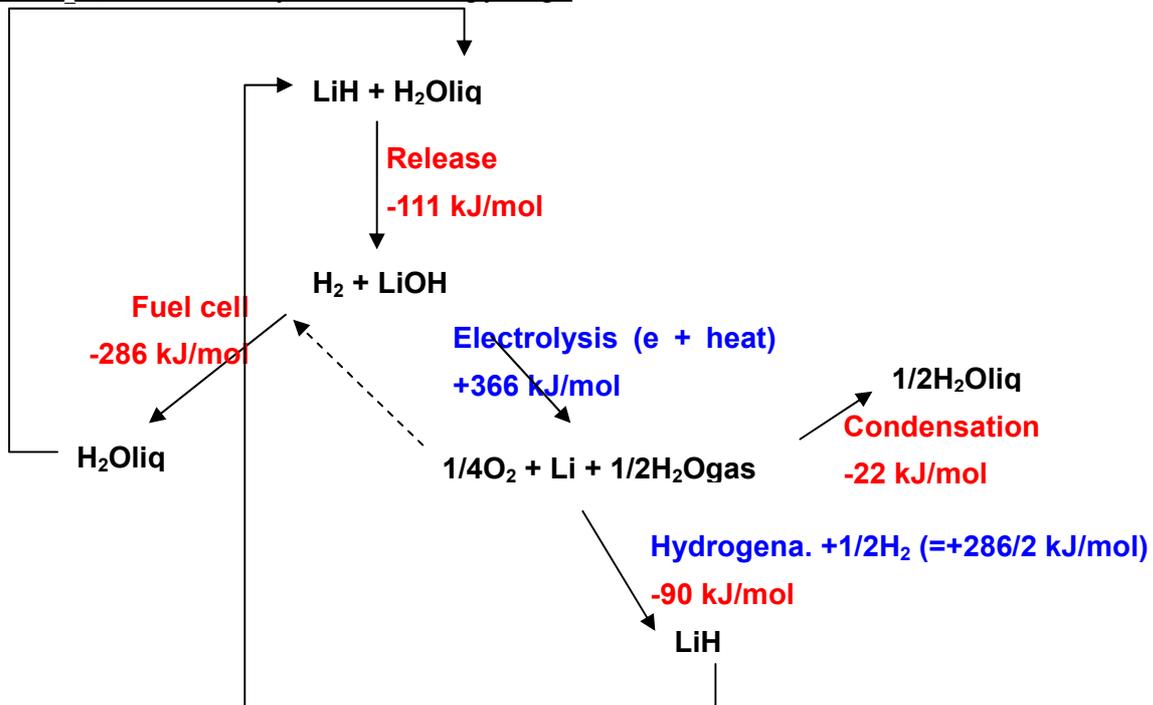
Li + H₂O, with electrolysis and enthalpy steps



Energetically, the H₂ supply system (release + electrolysis + condensation) is only filled with electricity (and heat) during the electrolysis.

Chemically, the global system (including the fuel cell) is chemically closed (O₂ may or may not be released to air during electrolysis). The global reaction is **electricity (+heat) --> electricity (+heat)**. It is therefore comparable to a battery, in principle.

LiH + H₂O, with electrolysis and enthalpy steps



Energetically, the H₂ supply system (release + electrolysis + condensation + hydrogenation) is filled both by H₂ and by electricity (and heat) during electrolysis.

Chemically, the global system (including the fuel) is not chemically closed. The global reaction is $1/2 \text{H}_2 + 1/4 \text{O}_2 + \text{electricity (+heat)} \rightarrow 1/2 \text{H}_2\text{Oliq} + \text{electricity (+heat)}$. Hence this system is in between a battery, and a fuel cell with storage, in principle.

3.3. Energy Efficiency (estimated on enthalpy, H, cycle)

The energy losses and gains in the system can be discussed from the variations of enthalpy (ΔH) for the compounds considered at same stoichiometry for each step. Enthalpy is directly interpretable as the energy of the system. In this first approach, we consider only standard conditions. This is not really correct, in particular for the electrolysis which is led at high temperatures.

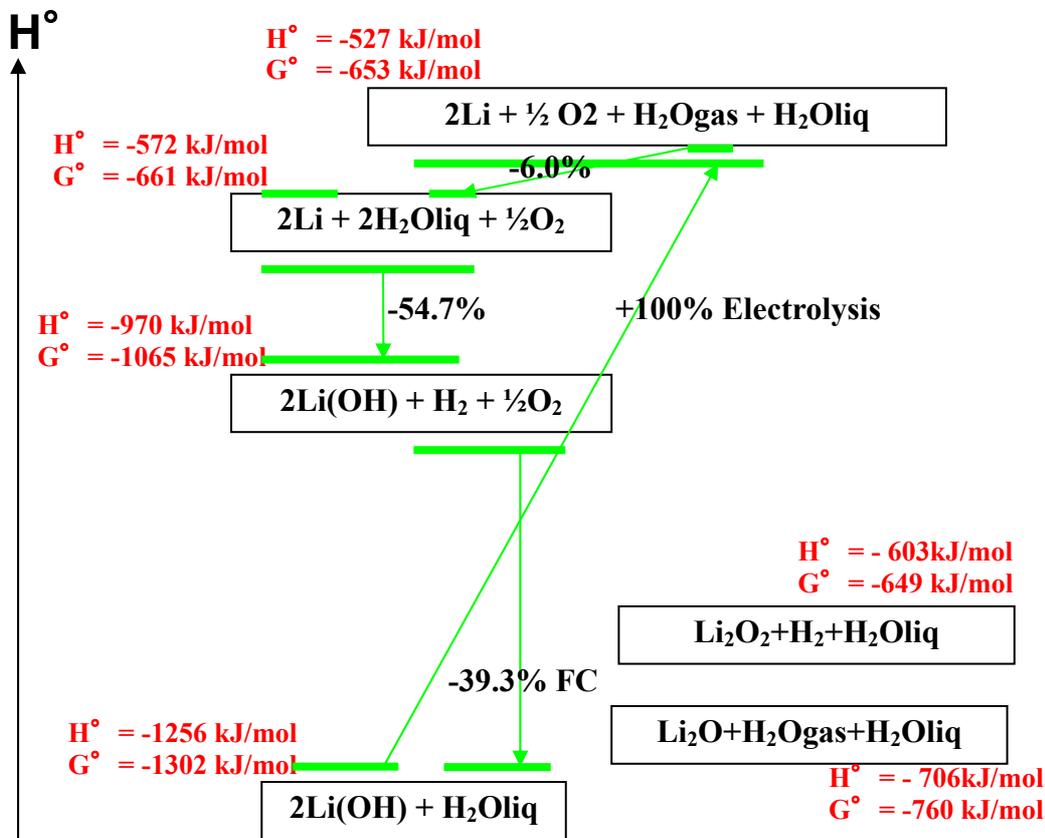
For the spontaneous steps, like hydrogenation or condensation, enthalpy difference is simply equal to the heat released.

For the fuel cell step, the enthalpy difference is the total energy given by the system. One part is given off as heat, and one part as useful electricity. The maximal electrical energy available considering entropy requirement is the difference in free energy, ΔG . However commercial fuel only produce about 50% of ΔG , or about 40% of ΔH , as electricity.

For the electrolytic step, the enthalpy difference is the total energy absorbed by the system. One part is absorbed as electricity, and one part is absorbed as heat from environment. Again, the minimal electrical energy to be input is the difference in free energy, ΔG (about 89% of ΔH for LiOH electrolysis at room temperature). Hence the electrolysis efficiency can theoretically be higher than 100% (up to 111% for LiOH at room temperature). In addition, this efficiency is expected to increase with temperature. However, a realistic estimation of the efficiency is difficult. It depends on heat loss from the system and on electrolysis temperature. For simplification we usually suppose 100% efficiency on the electrolytic step.

Li + H₂O, with electrolysis (Li₂O3H4 stoichiometry)

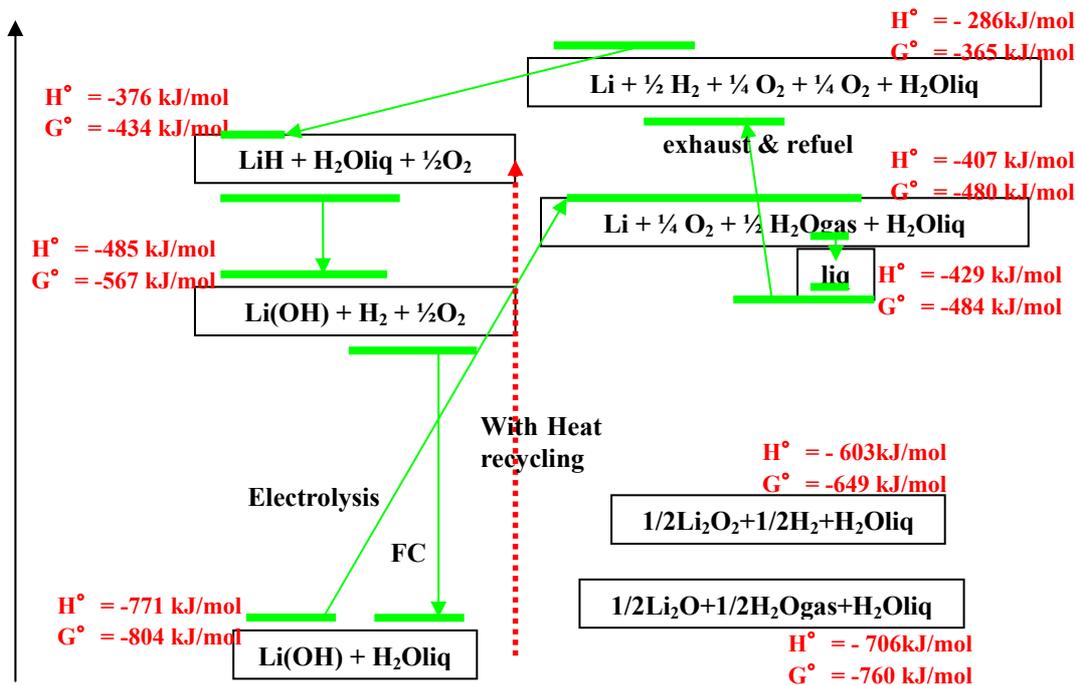
[We indicate the absolute values for enthalpy of formation and free energy of formation, and (in percent) the ratio of reaction enthalpy to energy input.]



The main loss in the storage system is due to hydrogen release reaction (54.7% relative to total energy input). Electrolysis is expected efficient. However, water condensation causes about 6% heat loss (recycling this heat from H₂O/O₂ gas exhaust is not possible in this case). Additional heat losses from the system exist but are difficult to quantify.

Li + H₂O efficiency (enthalpy based)		
Input (kJ/mol)	Filled (kJ/mol)	
727.970	683.970	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
44.000	398.140	
Filling efficiency	Release efficiency	Total efficiency
0.940	0.418	0.393

Note: "filling" includes electrolysis and water condensation. "release" includes only the hydrogen release step.

LiH + H₂O, with electrolysis (stoichiometry LiO₂H₃)


The main losses in the storage system are now:

- Li + 1/2 H₂ -> LiH (18% relative to total energy input)
- LiH + H₂O -> LiOH + H₂ (21% relative to total energy input)

In addition, and as in the previous case, there are losses from water condensation (4%) and from the system (difficult to quantify).

LiH + H ₂ O, Non heat-recycled efficiency (enthalpy based)		
Input (kJ/mol)	Filled (kJ/mol)	
506.900	394.400	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
112.500	108.570	
Filling efficiency	Release efficiency	Total efficiency
0.778	0.725	0.564

Note: "filling" includes electrolysis, water condensation, and hydrogenation. "release" includes only the hydrogen release step.

For the LiH system, it may be possible to recycle part of the heat lost by hydrogenation and water condensation to feed the endothermic electrolysis. This supposes that all steps in the filling (electrolysis + condensation + hydrogenation) are performed simultaneously (see part 3.5 for feasibility). Hopefully, we may get close to 100% energy efficiency on filling (at high temperature).

LiH + H₂O, Heat-recycled efficiency (enthalpy based)		
Input (kJ/mol)	Filled (kJ/mol)	
394.400	394.400	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
0.000	108.570	
Filling efficiency	Release efficiency	Total efficiency
1.000	0.725	0.725

3.4 Storage densities

Storage density of LiH is excellent, from 25.4%mass at reaction start to 8.4%mass at reaction end.

LiH is far superior to Li for storage density. The main reason is that LiH storage can provide one H₂ molecule for one H₂O molecule consumed, so that no storage of water is necessary. In contrast, the Li storage can provide only one H₂ molecule for two H₂O molecules consumed. Hence, half of the water must be stored.

2Li + 2 H₂Oliq -> H₂+2Li(OH) Storage Densities			
H ₂ Mass ratio at start [H ₂ /(2Li+ H ₂ O)]	0.063	H ₂ Mass ratio at end [H ₂ /(2LiOH)]	0.042
MJ/kg	8.961	MJ/kg	5.968
MJ/l	6.494	MJ/l	8.713
<i>ex: To store 7kg H₂, Li and H₂O at start (kg)</i>	110.765	<i>Li(OH) at end (kg)</i>	166.324
<i>Vol at start as liquid (l)</i>	152.833	<i>LiOH Vol at end as liquid (l)</i>	113.921
<i>Li mass fraction at start (kg)</i>	48.206	<i>H₂O mass fraction at start (kg)</i>	62.559
<i>Li vol fraction at start (l)</i>	90.274	<i>H₂O vol fraction at start (l)</i>	62.559

LiH + H₂Oliq -> H₂+Li(OH) Storage Densities			
H ₂ Mass ratio at start [H ₂ /(LiH)]	0.254	H ₂ Mass ratio at end [H ₂ /LiOH]	0.084
MJ/kg	35.958	MJ/kg	11.935
MJ/l	29.486	MJ/l	17.426
<i>ex: To store 7kg H₂, LiH at start (kg)</i>	27.603	<i>LiOH at end (kg)</i>	83.162
<i>Vol at start as liquid (l)</i>	33.662	<i>LiOH Vol at end as liquid (l)</i>	56.960
<i>Li mass fraction (kg)</i>	24.103		

3.5. Technical feasibility

Requirement for the electrolyser

- Resistance to 450C
- Resistance to highly basic LiOH

- Resistance to O₂, H₂O and H₂ corrosion
- Lightness
- Cheapness
- Mechanically resistance
- Well sealed

The materials commonly used in melted salt hydrolysis are graphite and steel (carbon coated).

Design of the electrolyser

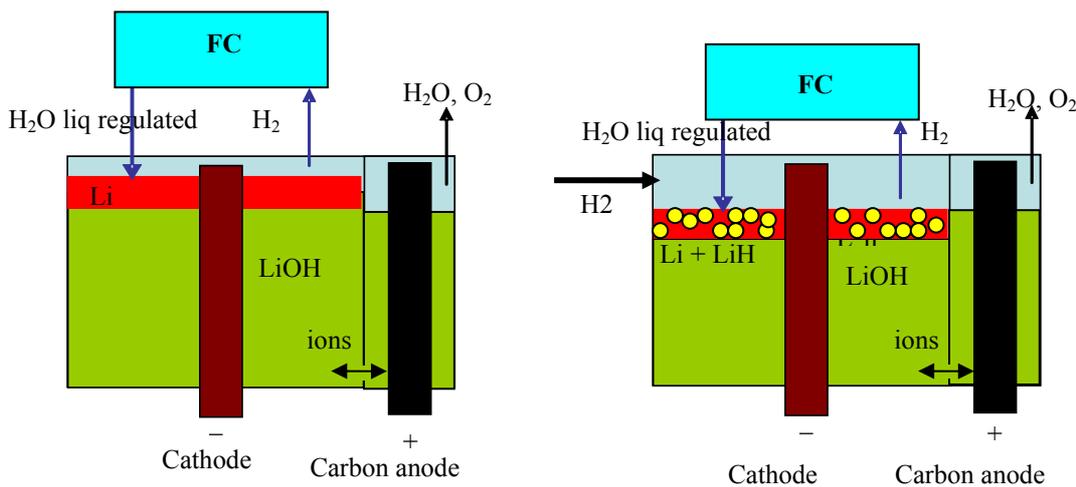
At the anode, H₂O and O₂ should be removed as gas exhaust. (The system should forbid that Li recombines with H₂O to give H₂ and LiOH. This would cause unnecessary heat loss.)

At the cathode, and in the LiH + H₂O system, it is favourable to have the electrolysis and the H₂ filling simultaneously, because:

1. Li -> LiH reaction heat could be used to warm the system, and feed the endothermic electrolysis.
2. Heat loss from water condensation could be transferred to H₂ input by thermal exchanger.
3. The heat delivered may be sufficient to melt LiOH without additional heating device.

Note: At high temperature, a reaction $LiOH + H_2 \rightarrow LiH + H_2O_{gas}$ may become spontaneous. This is to be checked. The contact surface between electrode and H₂ may play a role too by ionisation on the anode $H_2 \rightarrow 2H^-$, then $LiOH + H^- \rightarrow LiH + OH^-$

The figures below gives an example of a primitive design:



2Li + 2H₂O system(left) and LiH + H₂O system (right)

Chemical flows are indicated in blue for release, and in black for filling.

Tank and cathode materials may be carbon coated steel.

It is important to notice that the LiH system can work as a Li system and will do partially, when the hydrogenation reaction is incomplete.

4. Na/O/H based systems

4.1. Generalities

Stable compounds: Na, NaOH, Na₂O, (Na₂O₂), O₂, H₂O, H₂

Na melting (C)	98
NaH decomposition (C)	425
NaOH melting (C)	318
NaOH decomposition (C)	1390

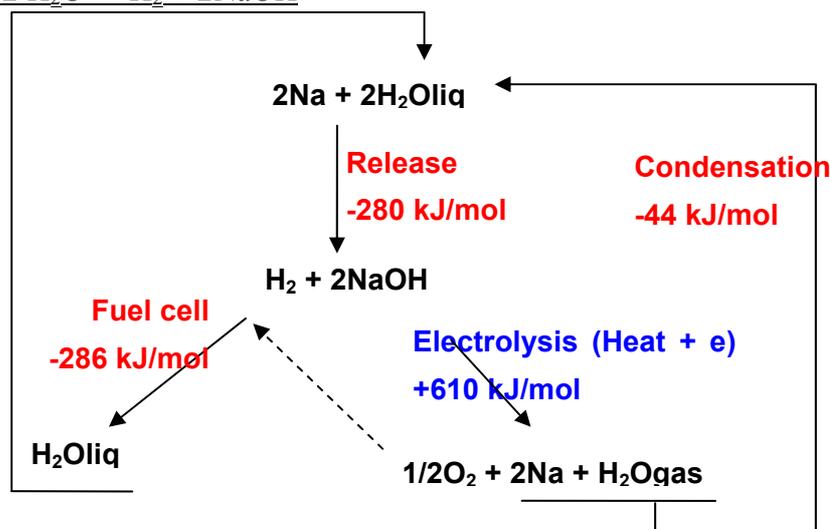
The Na/O/H system is very similar to the Li system. The advantages of Na compared to Li are:

- a higher energy efficiency on release thanks to a lower heat release during hydration
- a higher energy efficiency on filling, thanks to a lower heat release during hydrogenation, and to a lower electrolytic step
- a more reactive release thanks a higher water solubility of hydroxide and to a higher electropositivity
- A more practical electrolysis thanks to a larger range of temperatures where NaOH is liquid.

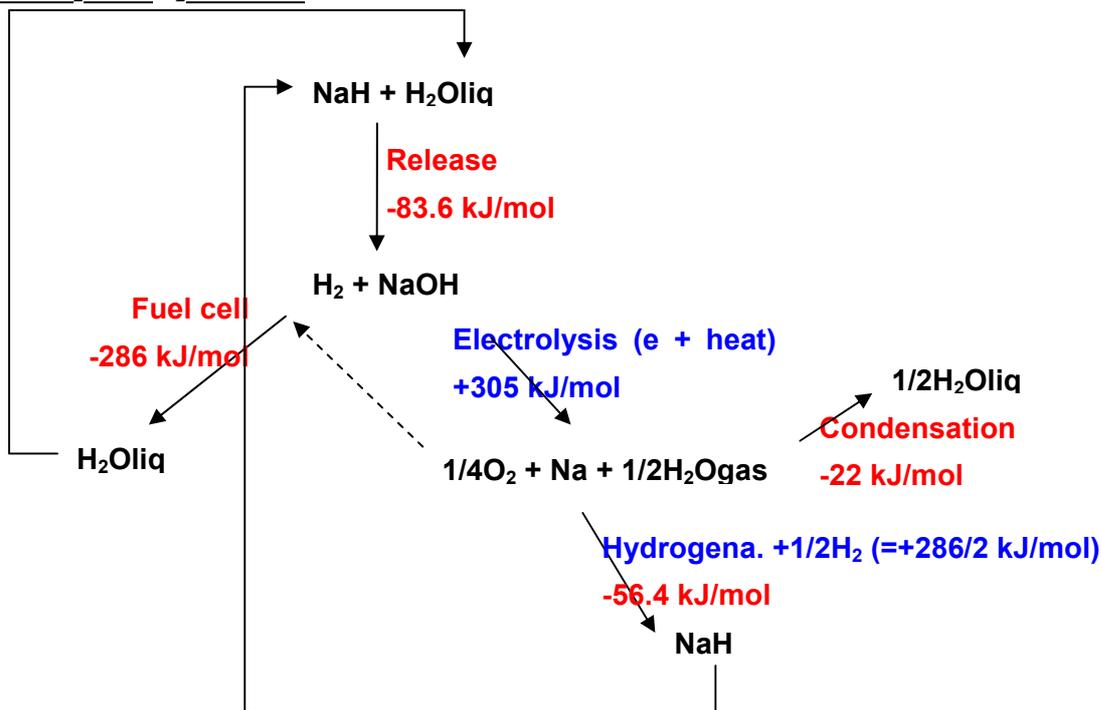
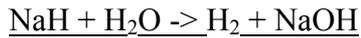
However, Na suffers from lower energy density, being 3 times heavier than Li.

Known actors on similar reactions: PowerBall technologies LLC [NaH in plastic ball storage, NaH+H₂O release, NaOH reduction by CH₄ at 980C]

4.2 Reaction pathway



Global reaction: **electricity (+heat) --> electricity (+heat)**. Chemically closed system



Global reaction: $1/2 \text{H}_2 + 1/4\text{O}_2 + \text{electricity (+heat)} \rightarrow 1/2 \text{H}_2\text{Oliq} + \text{electricity (+heat)}$

4.3. Energy Efficiencies

Na + H ₂ O efficiency		
Input (kJ/mol)	Filled (kJ/mol)	
609.370	565.370	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
44.000	279.540	
Filling efficiency	Release efficiency	Total efficiency
0.928	0.506	0.469

NaH + H ₂ O, Non heat-recycled efficiency		
Input (kJ/mol)	Filled (kJ/mol)	
447.600	369.300	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
78.300	83.470	
Filling efficiency	Release efficiency	Total efficiency
0.825	0.774	0.639

NaH + H₂O, Heat-recycled efficiency		
Input (kJ/mol)	Filled (kJ/mol)	
369.300	369.300	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
0.000	83.470	
Filling efficiency	Release efficiency	Total efficiency
1.000	0.774	0.774

4.4. Storage densities

2Na + 2 H₂Oliq -> H₂+2Na(OH) Storage Densities			
H ₂ Mass ratio at start [H ₂ /(2Na+ H ₂ O)]	0.031	H ₂ Mass ratio at end [H ₂ /(2NaOH)]	0.025
MJ/kg	4.466	MJ/kg	3.573
MJ/l	4.369	MJ/l	7.611
<i>ex: To store 7kg H₂, Na and H₂O at start (kg)</i>	222.226	<i>Na(OH) at end (kg)</i>	277.785
<i>Vol at start as liquid (l)</i>	227.164	<i>NaOH Vol at end as liquid (l)</i>	130.415
<i>Na mass fraction at start (kg)</i>	159.667	<i>H₂O mass fraction at start (kg)</i>	62.559
<i>Na vol fraction at start (l)</i>	164.605	<i>H₂O vol fraction at start (l)</i>	62.559

NaH + H₂Oliq -> H₂+NaOH Storage Densities			
H ₂ Mass ratio at start [H ₂ /(NaH)]	0.084	H ₂ Mass ratio at end [H ₂ /NaOH]	0.050
MJ/kg	11.911	MJ/kg	7.146
MJ/l	16.627	MJ/l	15.222
<i>ex: To store 7kg H₂, NaH at start (kg)</i>	83.334	<i>NaOH at end (kg)</i>	138.892
<i>NaH Vol at start as liquid (l)</i>	59.694	<i>NaOH Vol at end as liquid (l)</i>	65.208
<i>Na mass fraction (kg)</i>	79.834		

4.5. Technical feasibility

Systems are the same as for Li, except that the temperature involved may be different.

5. Na/B/O/H based systems (NaBH₄)

5.1. Generalities

(NaBH₄ is reviewed as there abundant literature. LiBH₄ or other similar compounds may be assumed of close behaviour.)

Stable compounds: Na, NaH, NaOH, Na₂O, B, B₂H₆, B(OH)₃, B₂O₃, NaBH₄, (NaB(OH)₄), NaBO₂, H₂O, H₂ (non exhaustive list)

NaBH₄ is interesting for:

- a high storage density
- a high release efficiency thanks to low heat loss on hydration $1/4\text{NaBH}_4 + 1/2\text{H}_2\text{O} \rightarrow \text{H}_2 + 4\text{NaBO}_2$
- a catalyst-activated release reaction
- a real water recycling rate of 100%, as the release reaction consumes only half a H₂O molecule per H₂ molecule released.

Unfortunately, there is also a major drawback from the fact that NaBO₂ is not easily or efficiency recycled (doubtful cyclability).

In addition:

- The reaction is slow without catalyst. And catalytic activity is impeded by insoluble NaBO₂ deposition on the catalysts.
- The high number of compounds causes side reactions. In particular there is probably the formation of the hydroxides: $\text{NaBH}_4 + 4 \text{H}_2\text{O} \rightarrow \text{NaOH} + \text{B(OH)}_3 + 4 \text{H}_2$

For these reason NaBH₄ is rather a compound for non-recycled storage where high energy cost is no issue.

Known actors: Millenium cell (Aude Cuni at CRCD is currently evaluating NaBH₄ technology as well, so this short review is not meant to be completely comprehensive.)

5.2. Reaction pathway

$1/4\text{NaBH}_4 + 1/2 \text{H}_2\text{O} \rightarrow \text{H}_2 + 4\text{NaBO}_2$ is a spontaneous reaction but slow at room temperature. It can be catalyst activated.

Non-recycled synthesis of NaBH₄:

- NaCl-electrolysis- $\rightarrow \text{Na} + \text{H}_2 \rightarrow \text{NaH} + \text{B(OCH}_3)_3 \rightarrow \text{NaBH}_4$ (low energetic efficiency)
- NaOH-electrolysis- $\rightarrow \text{Na} + \text{H}_2 \rightarrow \text{NaH} + \text{B(OCH}_3)_3 \rightarrow \text{NaBH}_4$ (millennium cell)

Recycling NaBO₂ to NaBH₄ is a major difficulty. It is not achieved today, and may never be with the requirement of high energetic efficiency and high purity. The fundamental problem lies in the complexity of a quadri-atomic system. We give below some routes studied at present.

High Temperature reduction (hypothetical reactions):

- $\text{NaBO}_2 + \text{ROH} + \text{CO}_2 \rightarrow \text{B(OR)}_3 + \text{Na}_2\text{CO}_3$; then $\text{B(OR)}_3 + \text{H}_2 \rightarrow \text{B}_2\text{H}_6 + \text{ROH}$; then $\text{B}_2\text{H}_6 + \text{Na}_2\text{CO}_3 \rightarrow \text{NaBH}_4 + \text{CO}_2$ (millennium cell)
- $\text{NaBO}_2 + 2\text{Mg} + 2 \text{H}_2 \rightarrow \text{NaBH}_4 + 2\text{MgO}$ (Merit)

Electrolysis (hypothetical reactions):

➤ $\text{NaBO}_2 + \text{H}_2\text{O} \rightarrow \text{Na} + \text{B}(\text{OH})_3 + \text{O}_2$; or $\text{NaBO}_2 + \text{H}_2 + \text{H}_2\text{O} \rightarrow \text{Na} + 4\text{B}(\text{OH})_3$ (millennium cell)

NaBH₄ + H₂O efficiency		
Input (kJ/mol)	Filled (kJ/mol)	
non viable	340.015	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
non viable	54.185	
Filling efficiency	Release efficiency	Total efficiency
non viable	0.841	non viable

5.3. Storage densities:

1/4NaBH₄ + 1/2H₂Oliq → H₂+1/4NaBO₂ Storage Densities			
H ₂ Mass ratio at start [H ₂ /(1/4NaBH ₄)]	0.213	H ₂ Mass ratio at end [H ₂ /(1/4NaBO ₂)]	0.123
MJ/kg	30.221	MJ/kg	17.376
MJ/l	32.458	MJ/l	42.815
<i>ex: To store 7kg H₂, NaBH₄ at start (kg)</i>	<i>32.843</i>	<i>NaBO₂ at end (kg)</i>	<i>57.122</i>
<i>NaH Vol at start as liquid (l)</i>	<i>30.580</i>	<i>NaOH Vol at end as liquid (l)</i>	<i>23.183</i>
<i>Na mass fraction (kg)</i>	<i>19.958</i>		
<i>B mass fraction</i>	<i>9.385</i>		

6. Higher hydrides (MH₂, MH₃)

6.1. Mg/O/H based systems

Stable Compounds: Mg, MgH₂, Mg(OH)₂, MgO, O₂, H₂O, H₂

Magnesium offers a good mass density (MgH₂ can reduce two water molecule. This compensate for the relatively high mass of Mg atom), and volumetric density.

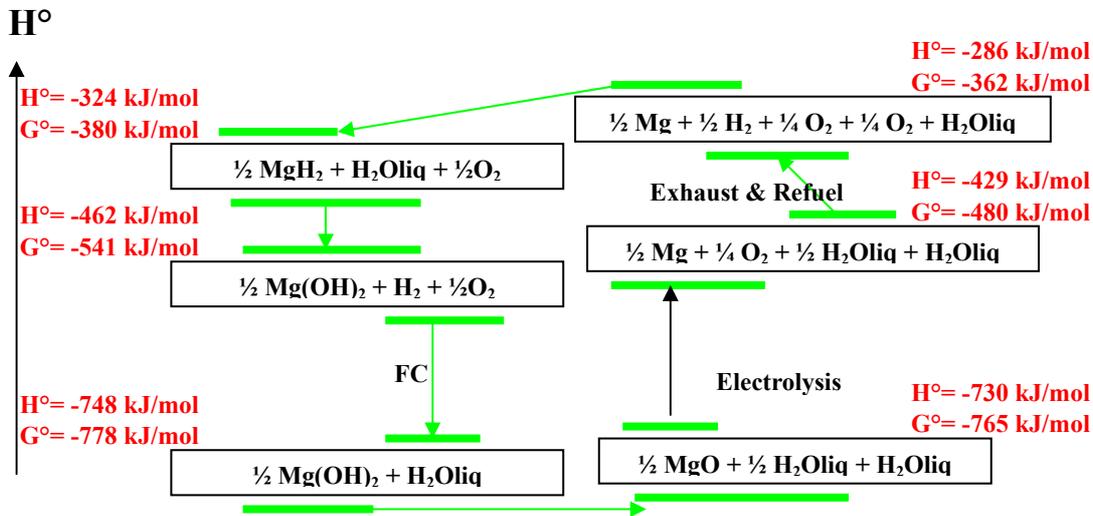
But it suffers from two problems:

- Hydroxide is rather unstable to the oxide. On moderate heating Mg(OH)₂ decomposes to MgO + H₂O. MgO can't be melted at low temperatures (melting at 2852C), and therefore melted salt electrolysis is not possible. Alternative "solid oxide membrane" electrolysis at 1200C has been proposed, but the efficiency of the process is uncertain (Safe hydrogen LLC).
- MgH₂ is little soluble in H₂O, hence H₂ release is expected slow or incomplete.

Known actors on similar reactions: Safe hydrogen LLC [MgH₂ slurry (mix with oil) storage, MgH₂+ H₂O release, SOM electrolysis recycling]

Reaction pathway and efficiency

(iso-stoichiometry $1/2\text{MgO}_2\text{H}_3$):



MgH ₂ + H ₂ O, Heat-recycled efficiency		
Input (kJ/mol)	Filled (kJ/mol)	
non viable	424.255	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
non viable	138.425	
Filling efficiency	Release efficiency	Total efficiency
non viable	0.674	non viable

Storage density

1/2MgH ₂ + H ₂ Oliq -> H ₂ +1/2Mg(OH) ₂ Storage Densities			
H ₂ Mass ratio at start [H ₂ /(1/2MgH ₂)]	0.153	H ₂ Mass ratio at end [H ₂ /(1/2Mg(OH) ₂)]	0.069
MJ/kg	21.719	MJ/kg	9.802
MJ/l	31.492	MJ/l	23.133
ex: To store 7kg H ₂ , Mg H ₂ at start (kg)	45.700	Mg(OH) ₂ at end (kg)	101.259
Vol at start as liquid (l)	31.517	Vol at end as liquid (l)	42.907
Mg mass fraction (kg)	42.200		

6.2. Be/O/H based systems

Stable Compounds: Be, BeH₂, Be(OH)₂, BeO, O₂, H₂O, H₂

The Be/O/H system is very similar to the Mg/O/H system. But, beryllium being much lighter than magnesium, it enables the highest storage density of all compounds studied here (up to 36% mass!).

However there is an important drawback from the fact that Be compounds are very toxic (carcinogenic).

In addition, beryllium suffers of the same problems than magnesium:

- the hydroxide is instable to the oxide (possibly at room temperature)
- the hydroxide is little soluble

Reaction pathway

The reactions above can be used by replacing Mg with Be, with very little change on energy levels.

BeH₂ + H₂O, Heat-recycled efficiency		
Input (kJ/mol)	Filled (kJ/mol)	
non viable	413.175	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
non viable	127.345	
Filling efficiency	Release efficiency	Total efficiency
non viable	0.692	non viable

Storage density

1/2BeH₂ + H₂Oliq -> H₂+1/2Be(OH)₂ Storage Densities			
H ₂ Mass ratio at start [H ₂ /(1/2MgH ₂)]	0.366	H ₂ Mass ratio at end [H ₂ /(1/2Mg(OH) ₂)]	0.094
MJ/kg	51.837	MJ/kg	13.286
MJ/l	33.002	MJ/l	25.509
<i>ex: To store 7kg H₂, Be H₂ at start (kg)</i>	<i>19.148</i>	<i>Be(OH)₂ at end (kg)</i>	<i>74.707</i>
<i>Vol at start as liquid (l)</i>	<i>30.076</i>	<i>Vol at end as liquid (l)</i>	<i>38.910</i>
<i>Be mass fraction (kg)</i>	<i>15.648</i>		

6.3. Al/O/H based systems

Stable Compounds: Al, AlH₃, Al(OH)₃, AlOOH, Al₂O₃, Al₂O, H₂, H₂O, O₂ (The trivalent character of Al³⁺ causes the existence of an additional compound AlOOH in the system.)

Aluminium offers a good mass storage density (AlH₃ reduces 3 water molecules. This compensate for the relatively high mass of Al atom.) and the best volumetric density of compounds studied here.

The release reaction $1/3\text{AlH}_3 + \text{H}_2\text{O} \rightarrow 1/3\text{Al(OH)}_3 + \text{H}_2$ is reported. (Al(OH)₃ and AlOOH are insoluble, but on the other hand Al is very electropositive.) But the low stability of the hydroxide may not allow efficient electrolysis, as in the case of Mg

The thermodynamic literature being incomplete for this family (for Al(OH)₃ in particular), we can not make a complete thermodynamic analysis here.

Storage density

1/3AlH₃ + H₂O -> 1/3Al(OH)₃ + H₂ Storage Densities			
H ₂ Mass ratio at start [H ₂ /(1/3AlH ₃)]	0.202	H ₂ Mass ratio at end [H ₂ /(1/2Mg(OH) ₂)]	0.078
MJ/kg	28.578	MJ/kg	10.993
MJ/l	45.153	MJ/l	26.603
<i>ex: To store 7kg H₂, AlH₃ at start (kg)</i>	<i>34.732</i>	<i>Al(OH)₃ at end (kg)</i>	<i>90.291</i>
<i>Vol at start as liquid (l)</i>	<i>21.982</i>	<i>Vol at end as liquid (l)</i>	<i>37.310</i>
<i>Al mass fraction (kg)</i>	<i>31.232</i>		

7. Li/N/H based system (non H₂O case)

7.1. Generalities

Stable Compounds: Li, LiH, Li₂NH, LiNH₂, Li₃N, N₂, NH₃, H₂ [N replaces O as the electronegative element of the system. Such a system allows one more compound because of trivalent bounded N³⁻ (compared to divalent O²⁻): Li₂NH and LiNH₂ instead of LiOH]

LiH melting (C)	680
Li ₃ N melting (C)	840-850
Li ₂ NH melting (C)	Unknown but in between
LiNH ₂ melting (C)	380-400
NH ₃ standard vapor pressure (bar)	8.8

The system is interesting for:

- a high storage density (even if water is not recycled from the fuel cell)

- a low heat loss on filling
- an original 3-steps reversible release/filling
- an endothermic release (may enable on board heat recycle)
- the use of NH₃ that is odour detectable

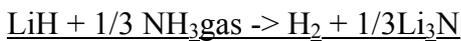
However it suffers of major drawbacks too:

- One of release steps (Li₂NH + LiH → H₂ + Li₃N) is probably not viable because the reactants are solids under 400C
- There is need for a separate pressurised NH₃ storage if NH₃ is used as fuel, hence storage density is greatly reduced.

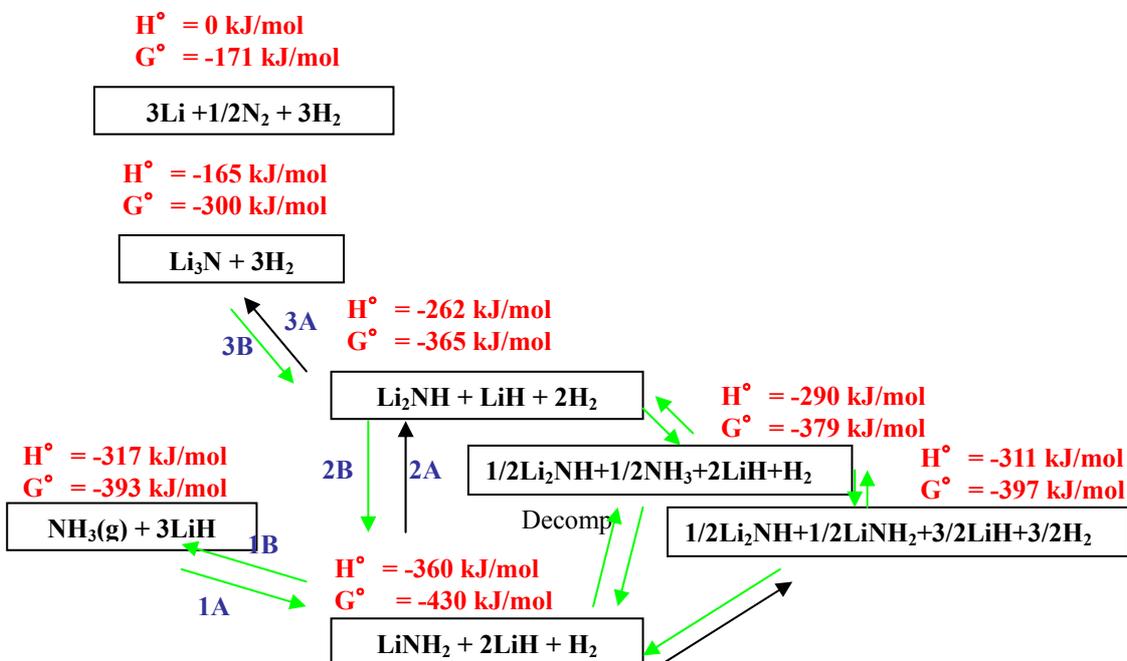
In addition:

- Two gases are involved (H₂ and NH₃), which means that gas separation is needed
- There is a risk of NH₃ pollution in the hydrogen input of the fuel cell
- No humidity can be provided to the hydrogen input of the fuel cell
- Li₃N is hydrophilic (Li₃N + 3 H₂O → 3LiOH + NH₃, enthalpy -485kJ/mol)

7.2. Reaction pathways



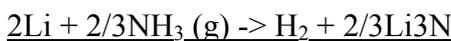
(iso-stoichiometry Li₃NH₆):



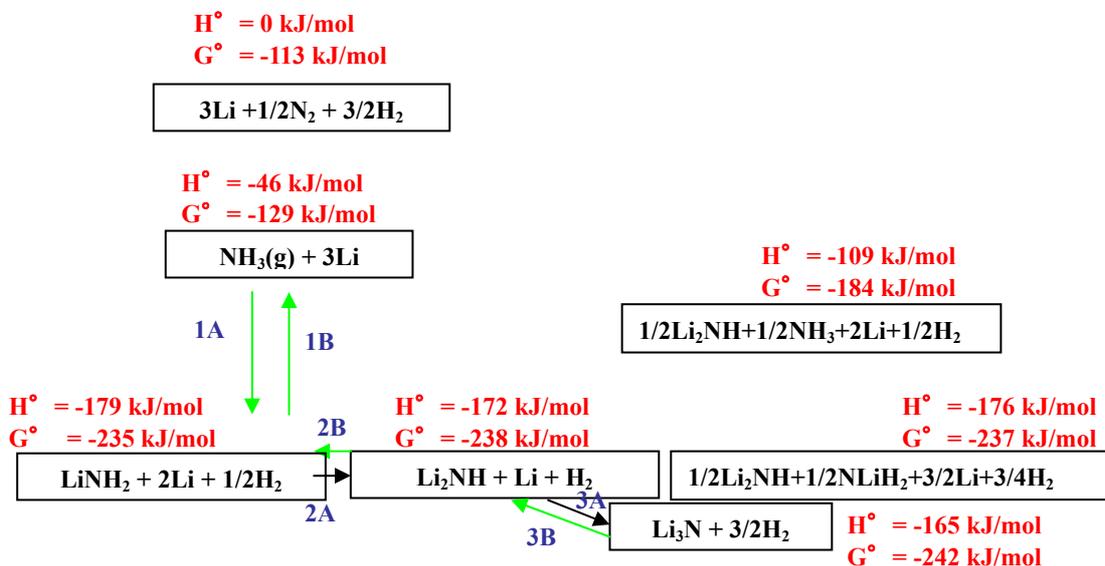
As shown above H₂ storage/release may proceed in many reactions and their combinations. Main are 1 2 3, each releasing or storing one H₂ molecule, hence each with a storage potential of about 5.5% mass. To have a useful storage system, we need 1+2, or 2+3, or better 1+2+3. The reactions

are expected to be reversible because the free energy steps between reactions are modest.

LiH + NH₃ (steps 1+2+3) efficiency		
Input (kJ/mol)	Filled (kJ/mol)	
1,010.330	857.490	
Loss on filling (kJ/mol)	Loss on release (kJ/mol)	
152.840	0.000	
Filling efficiency	Release efficiency	Total efficiency
0.849	1.000	0.849



(iso-stoichiometry Li₃NH₃):



These reactions are not really meaningful. It should be noted that all the products above have higher free energy of formation, G°, than their counterpart in the previous LiH system. [To compare with previous system at same stoichiometry, one can add 3/2H₂ and hence reduce G° of G°(3/2H₂)=-58.5 kJ/mol.] This means that the reaction between Li and H₂ is always the most favourable thermodynamically. Therefore the filling reactions are not viable. Filling with large amount of H₂ would lead to the LiH system.

In addition, the release reactions are only possible if H₂ does not react directly with Li. This reaction is reduced by:

- Removal of H₂
- Large dominance of NH₃ over Li

7.3. Storage densities

2Li+2/3NH₃ (g)-> H₂+2/3Li₃N Storage Densities			
H ₂ Mass ratio at start [H ₂ /(2Li+2/3NH ₃)]	0.080	H ₂ Mass ratio at end [H ₂ /(2/3Li ₃ N)]	0.087
MJ/kg	11.326	MJ/kg	12.310
MJ/l	6.363	MJ/l	16.003
<i>ex: To store 7kg H₂, at start (kg)</i>	<i>87.632</i>	<i>Li₃N at end (kg)</i>	<i>80.632</i>
<i>Vol at start as liquid (l)</i>	<i>155.984</i>	<i>Li₃N Vol at end as liquid (l)</i>	<i>62.025</i>
<i>Li mass fraction at start (kg)</i>	<i>48.206</i>	<i>NH₃ mass fraction at start (kg)</i>	<i>39.426</i>
<i>Li vol fraction at start (l)</i>	<i>90.274</i>	<i>NH₃ vol fraction at start (l)</i>	<i>65.710</i>

LiH+1/3NH₃ (g)-> H₂+1/3Li₃N Storage Densities			
H ₂ Mass ratio at start [H ₂ /(LiH+1/3NH ₃)]	0.148	H ₂ Mass ratio at end [H ₂ /(1/3Li ₃ N)]	0.174
MJ/kg	20.977	MJ/kg	24.620
MJ/l	14.922	MJ/l	32.005
<i>ex: To store 7kg H₂, at start (kg)</i>	<i>47.316</i>	<i>Li₃N at end (kg)</i>	<i>40.316</i>
<i>Vol at start as liquid (l)</i>	<i>66.517</i>	<i>Li₃N Vol at end as liquid (l)</i>	<i>31.012</i>
<i>LiH mass fraction at start (kg)</i>	<i>27.603</i>	<i>NH₃ mass fraction at start (kg)</i>	<i>19.713</i>
<i>LiH vol fraction at start (l)</i>	<i>33.662</i>	<i>NH₃ vol fraction at start (l)</i>	<i>32.855</i>
<i>Li mass fraction (kg)</i>	<i>24.103</i>		

7.4. Technical feasibility

Important consideration for feasibility of a storage system:

1. If NH₃ is the storage material, NH₃ will be liquefied for high volumetric density. (NH₃ vapour pressure is 8.8 bar in standard conditions) However this storage should be kept from overheating in the reactor as the pressure would quickly rise on heating. (For instance, at 100C NH₃ vapour pressure is 60bar). This will reduce volumetric density.

2. Reactions where two reactants are solid (2A, 3A, black arrows) will proceed slowly and incompletely for the lack of contacts between reactants. This is a major concern. However:

- Starting from 1A, LiH is the only solid compound. If 1A, 2A and 3A are led at once, solids compounds may be in contact naturally.
- For reaction 2A, there is an alternative route through the decomposition of LiNH₂ (right side).

3. Endothermic reactions (1B, 2A and 3A) must be accelerated:

- Reactor temperature must be in the range 200-400C, which causes system difficulties and heat losses
- 1B must be accelerated by removing NH₃ (without removing H₂). We can use condensation or a

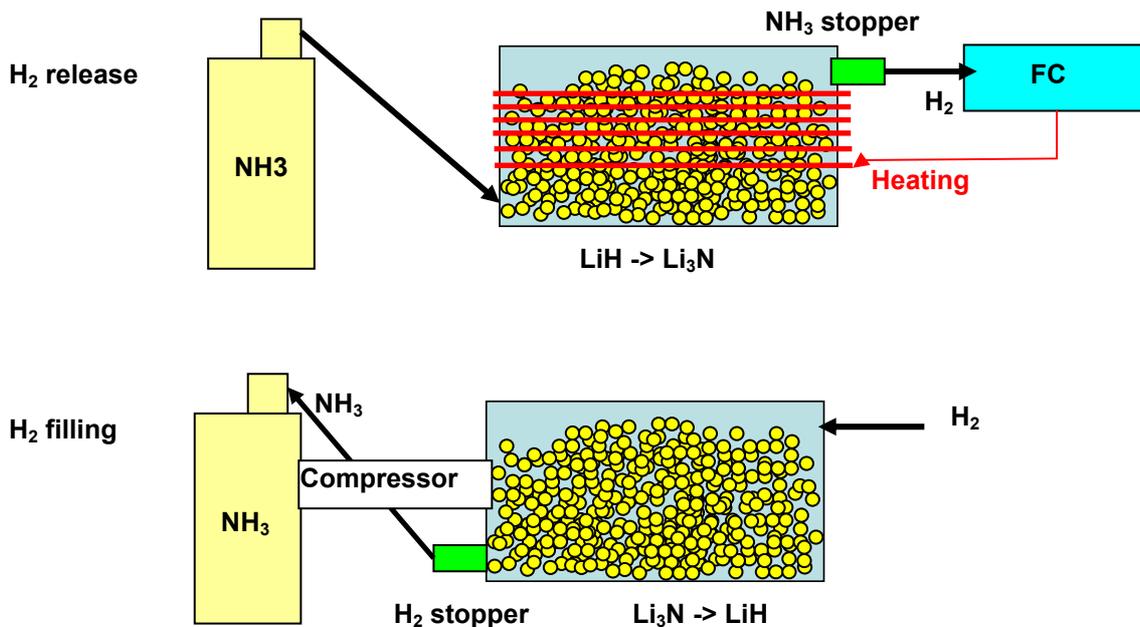
membrane separator or a water washing.

- 2A and 3A must be accelerated by removing H_2 (without removing NH_3). We can use condensation or a membrane separator. (For 1A separation between H_2 and NH_3 is useful too.)
- Pressure should be low in reactor

4. The release of H_2 is endothermic, so we may recycle heat from the system.

System design

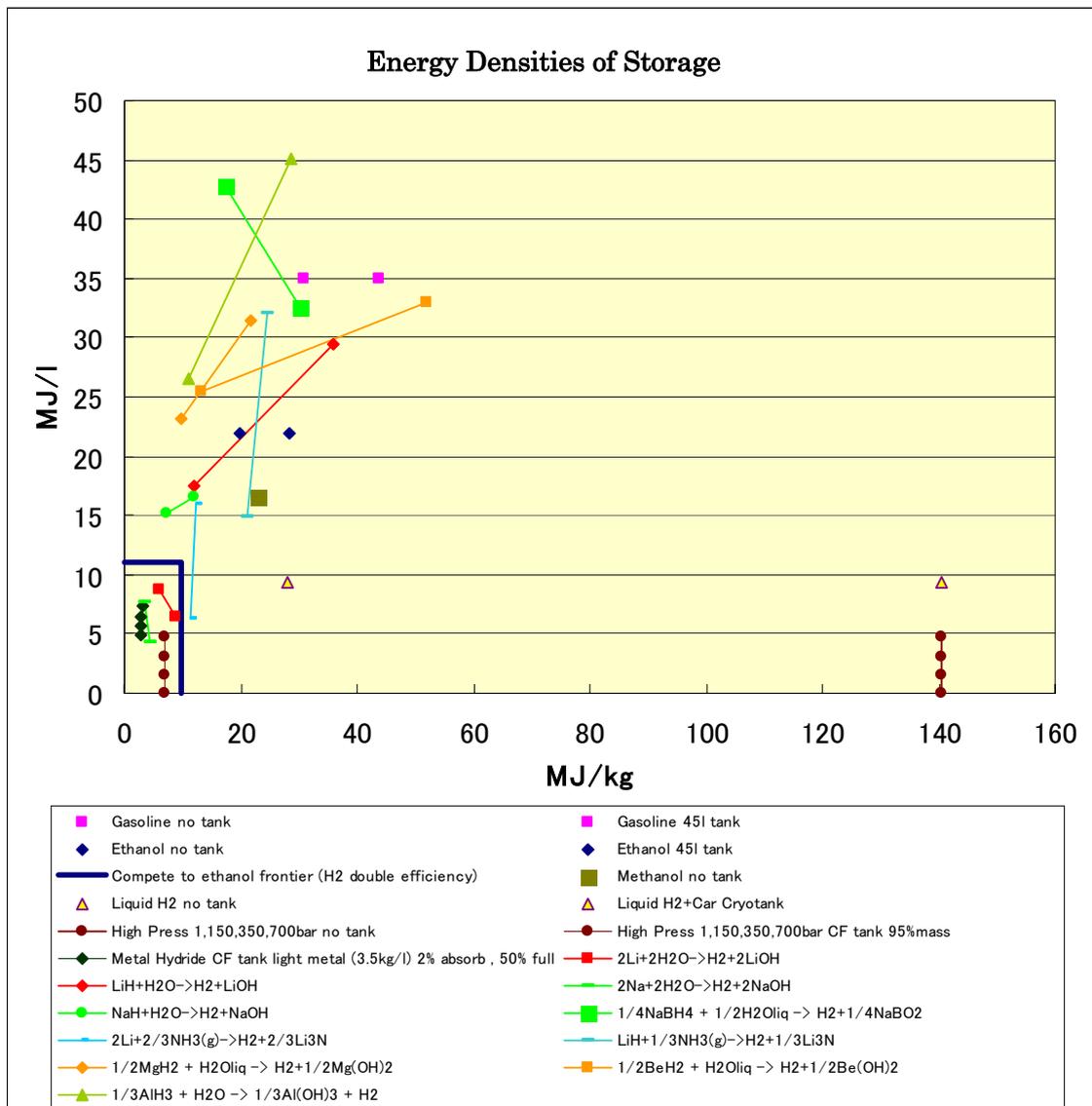
With the consideration above, we can deduce that NH_3 storage and reactor must be separated because there are incompatible requirements for these two steps regarding the temperature and pressure. This constraint consequently reduces the volumetric density by a factor of 2. In addition, we can expect a mass density reduction due to the mass of the compressed gas NH_3 cylinder (estimated as ~ 28 kgs for the cylinder to store 7 kgs of NH_3 based upon currently used CGA cylinders for NH_3 delivery).



8. Comparison

8.1. Energy density

The chart below presents a comparison of the studied systems from the point of view of energy densities (mass and volume). It also includes high pressure cylinders, liquid hydrogen tanks, metal hydride storage, as well as some hydrocarbon storages. LiH, MgH₂, BeH₂, AlH₃, and NaBH₄ offer a potential of storage density far above existing storage for hydrogen, and may be competitive to gasoline (considering the increased efficiency of a fuel cell with an electric motor to a thermal motor). NaH, LiH + NH₃, Li and Na have a somehow lower potential, but are still competitive with existing hydrogen storage.



Notes: Chemical storage values indicate supplied energy (heat losses on release have been taken into account). The values of volume density of chemical storage are idealistic. We do not take into

account the loss of volume density due to powder voids (volume as liquid) or of the system. Also, the values for mass densities should be corrected by the real loss of water in the fuel cell. For NH₃ reactions (sky blue), both densities may reduced of as much as a factor two, due to the requirements of a NH₃ cylinder storage.

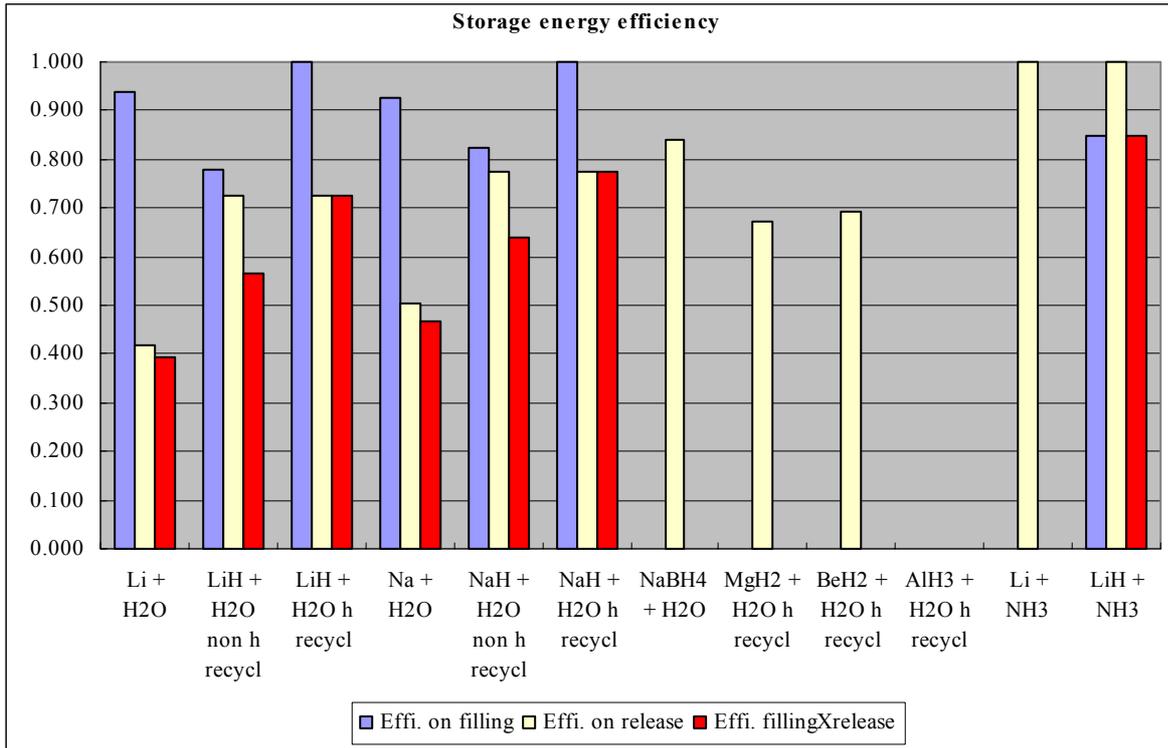
8.2. Storage efficiency

For release efficiency, LiH, MgH₂, BeH₂, AlH₃, and NaBH₄ have similar potentials between 65% and 85%, which are directly related to heat loss on hydration reaction. The release with Li and Na metals is less efficient (40 to 50%). An endothermal release, as in reactions with NH₃, offers of course a much higher efficiency potential, but reactivity is uncertain. The efficiency on release considers the amount of thermal energy that is lost due to the reaction generating the H₂. In other words the release efficiency is:

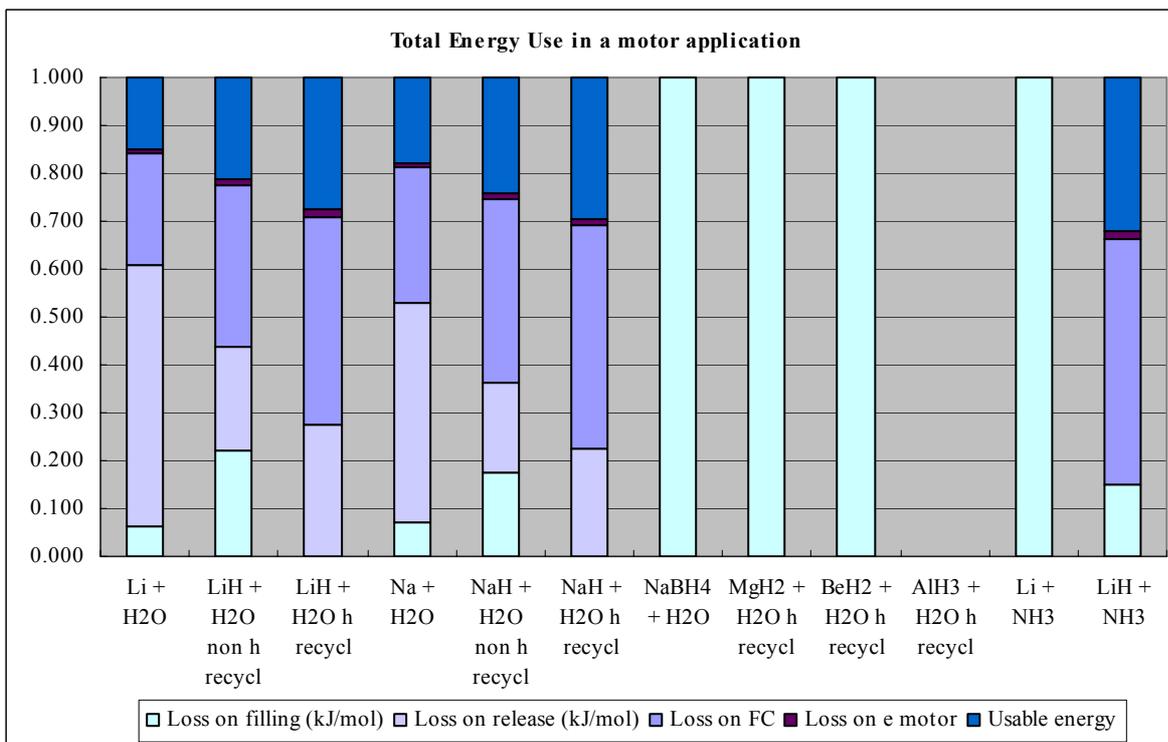
$$E = \frac{H_2 \text{ energy produced}}{H_2 \text{ energy produced} + \text{enthalpy of reaction}}$$

For filling efficiency, the figures are highly dependent on the possibility and on the efficiency of the melted salt electrolysis. Sodium and lithium compounds are the only compounds where a reasonable efficiency can be foreseen, between 75 and 100%. The feasibility and efficiency of the electrolysis is yet to be demonstrated experimentally however and is one of the critical evaluations necessary for final feasibility.

All in all, the potential energy efficiency of a cyclable storage with NaH or LiH is about 70%, hence an added cost of the storage of about 30%. This is comparable to the energy efficiency of a cryogenic storage for instance.



Considering an application including storage, fuel cell and electric motor (graph below), the total energy efficiency from energy input to mechanical energy could be up to 30% for LiOH and NaOH systems. This is better than usual gasoline combustion engine values of 20%. In other words, to be cost competitive, the input energy (hydrogen + electricity) for the chemical storage should be at most 50% more expensive than gasoline energy.



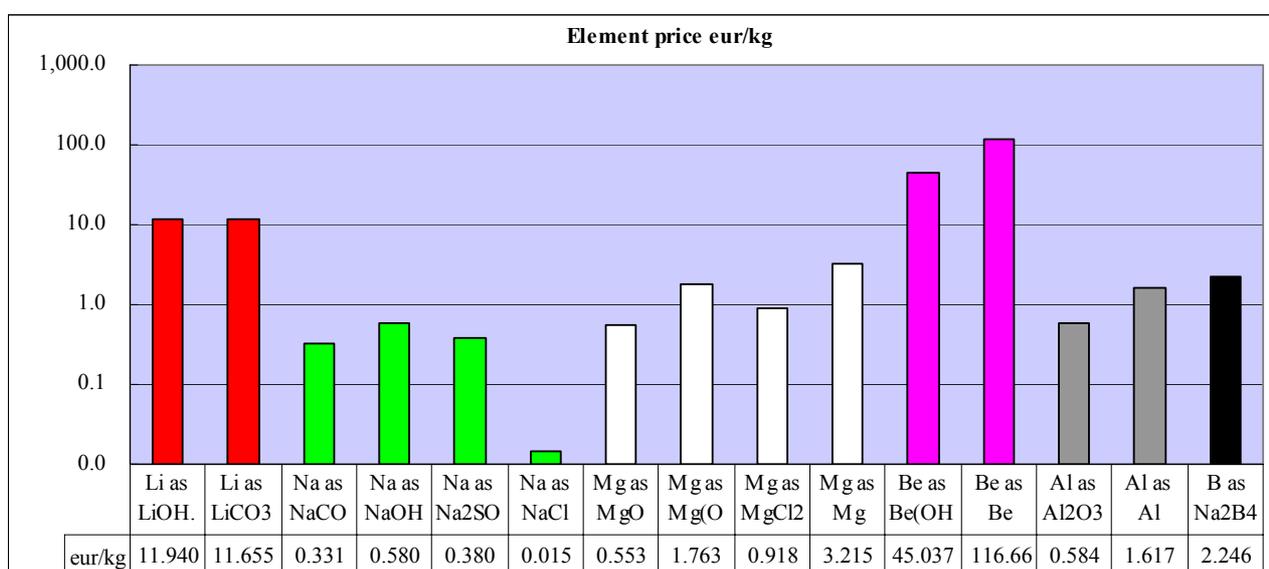
Notes: Fuel cell efficiency is supposed 40% of the enthalpy of combustion $H_2 + 1/2O_2 \rightarrow H_2O_{liq}$ (286

kJ/mol at 20C), ie ~50% of the free energy of combustion (Axane FC case). For $\text{NaBH}_4 + \text{H}_2\text{O}$, $\text{Li} + \text{NH}_3$, $\text{MgH}_2 + \text{H}_2\text{O}$, and $\text{BeH}_2 + \text{H}_2\text{O}$, an efficient filling/recycling is not determined. For $\text{AlH}_3 + \text{H}_2\text{O}$ the literature data is incomplete.

8.3. Element prices and availabilities

(Most data is from US geological survey <http://minerals.usgs.gov/minerals/pubs/commodity/>)

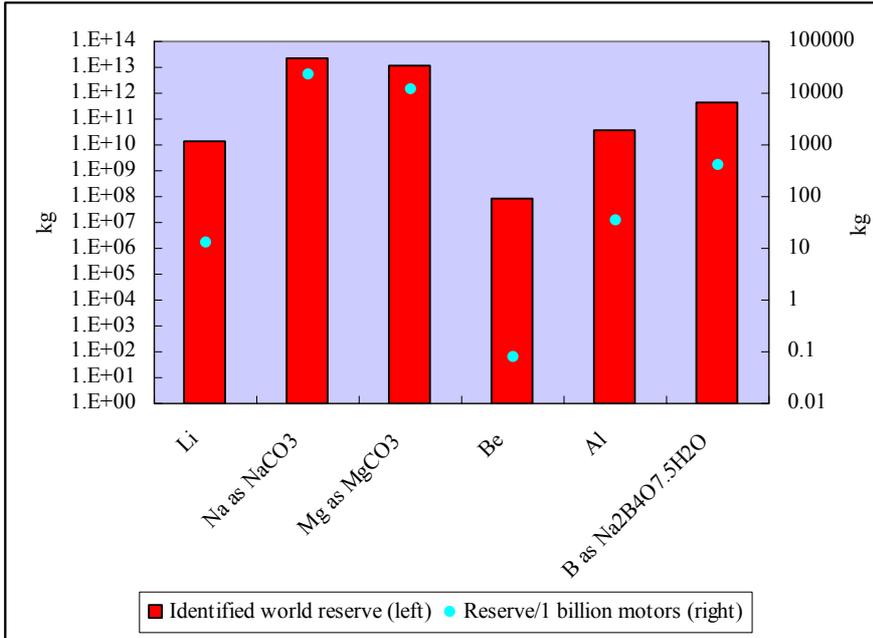
Metal prices (graph below) greatly differ between metals, from the very affordable sodium to the high valued beryllium. Lithium is a relatively expensive metal, roughly 20 times the price of sodium on same weight base.



Notes: Prices are calculated as (price of the compound)x(metal mass/compound mass). The costs of Li, Na and B as raw metals are not meaningful because markets are not significant. We expect cheap electrolytic reprocessing from hydroxide for Li and Na. On the opposite, B is obtained through an expensive reduction process with Mg at high temperature. Quotes as high as 2000\$/kg for amorphous B are found. NaOH (caustic soda) price has been highly fluctuant in last years due to changes in chlorine market.

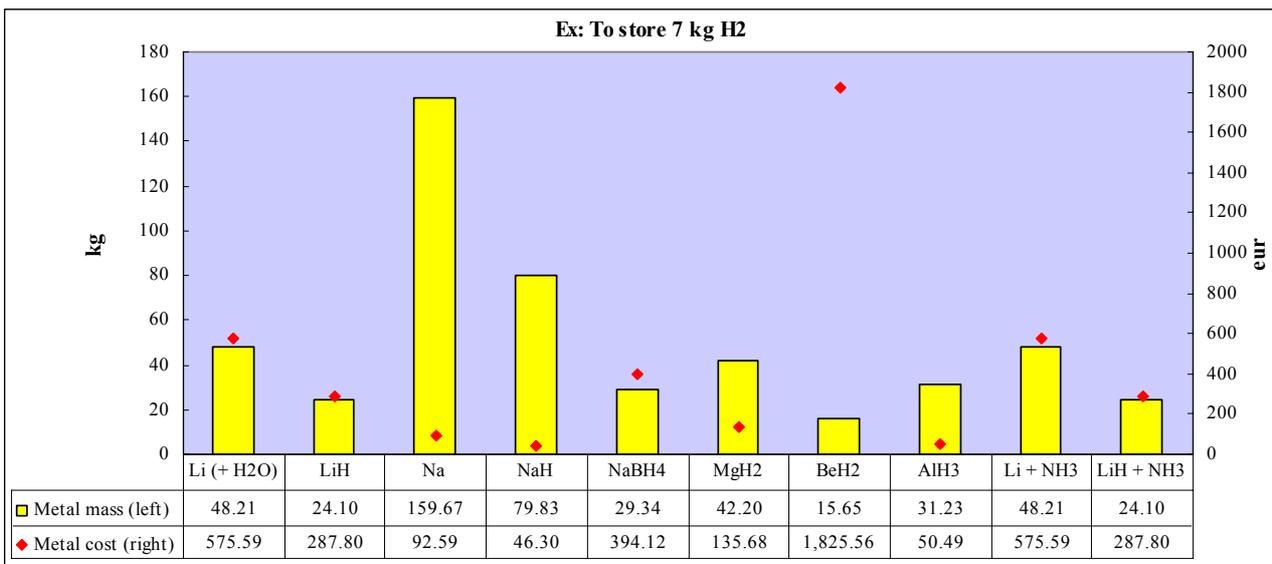
Metal price is not only determined by natural reserves (graph below), but also by the efficiency of the isolation process. For instance, aluminium is cheap thanks to a relatively efficient electrolytic isolation process from the oxide, but it is not an abundant resource. On the opposite, magnesium is a relatively expensive metal, although it is an abundant resource.

The reserves are very abundant for sodium and magnesium and scarce for beryllium. Again lithium is a relatively rare compound. The known world reserve amount would provide about 20kg of lithium for 1 billion motors (graph below, right scale).



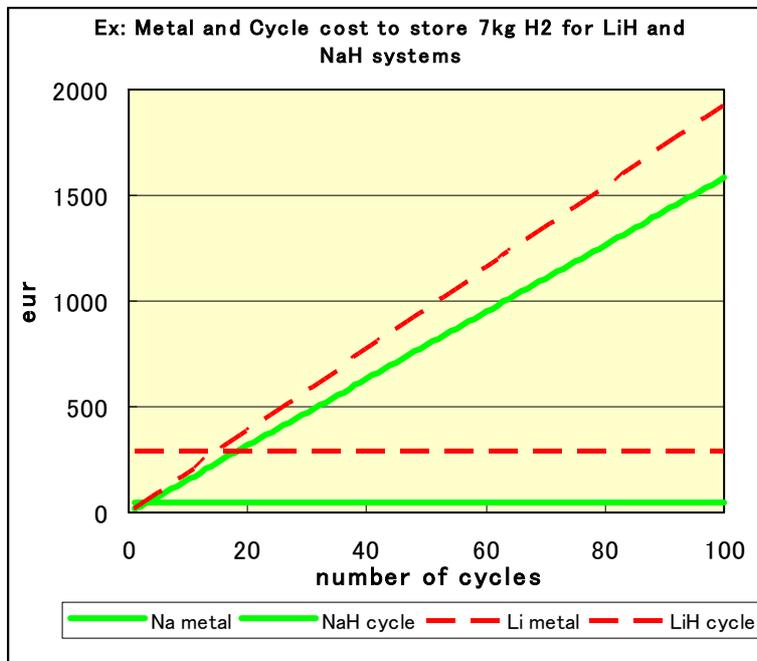
Note: Na from NaCl is not represented but virtually unlimited

To estimate the material cost in a storage system it should also be considered the mass of metal needed for each system. In the graph below, we ponder metal cost with metal mass needed to store 7kg of hydrogen. This considered, NaH and AlH₃ systems offer the cheapest metal cost. The price of lithium in a LiH type system is about 6 times higher than the equivalent price for sodium. The price of NaBH₄ in a NaBH₄ type system is about 8.5 times higher than the equivalent price for sodium.



Note: lithium and sodium costs are based on the hydroxide price. NaB cost is based on the minimal NaBH₄ price as estimated by an Air Liquide internal study of K. Barral. Others costs are based on the raw metal price.

Finally, it should be understood that, for highly cyclable systems, the cost of the metal is negligible compared to the cost of heat losses on the cycle after a number of cycles (graph below). For sodium, the metal cost is negligible if cyclability is above about 10 times. For lithium, the metal cost is negligible if cyclability is above about 100 times.



Note: Input energy cost is rounded to 10 eur per stored hydrogen kg.

If such high cyclability is obtained, the cost difference between systems is mostly determined by the energy efficiency on the cycle. In that case, and with the estimated efficiency of respectively 72% and 77% for LiH and NaH systems (part 8.2), the overcost of lithium to sodium is +22%.

9. Conclusions

	$Li + H_2O$	$LiH + H_2O$	$LiH + H_2O$ h-recycl	$Na + H_2O$	$NaH + H_2O$ h-recycl	$NaBH_4 + H_2O$	$MgH_2 + H_2O$ h-recycl	$BeH_2 + H_2O$ h-recycl	$AlH_3 + H_2O$ h-recycl	$Li + NH_3$	$LiH + NH_3$
Energy density	~	O	O	~	~	O	O	O	O	X	~
Filling effi.	O	~	O	O	O	X	X	X	?	X	~
Release effi.	~	O	O	~	O	O	O	O	?	O	O
Input energy	e + h	e + h + H ₂	e + h + H ₂	e + h	e + h + H ₂	NaB H ₄	Mg + H ₂	Be + H ₂	Al + H ₂	H ₂ + h	H ₂ + h
Metal price	~	~	~	O	O	~	O	X	O	~	~
Security	O	O	O	O	O	O	O	O	O	~	~
Environmental impact	O	O	O	O	O	O	O	X	O	O	O

Merits and demerits of each system: O for no-issue yet, X for major issue, ~ minor issue, e for electricity, h for heat

Cycled chemical storage using light metal hydrides offers a potential for storage and transport applications due to the remarkable energy density and reasonable energy efficiency potential (comparable to that of cryogeny for instance). Applications could be various, including long range distribution and automotive. From the present report we conclude that sodium and lithium may have the potential to be cycled with an energy-efficient electrolysis, provided feasibility is demonstrated experimentally. $LiH + H_2O$ and $NaH + H_2O$ based storages with carefully heat recycling could offer an energy efficiency up to about 70%, and an energy density far above that of other hydrogen storage methods. In terms of energy density, lithium potential is about twice that of sodium (for the filled tank). However, sodium is less expensive and more energy efficient on use than lithium. If high cyclability is achieved (over 100 cycles) the over-cost of lithium to sodium would be on the order of 22%.

Chemical hydrides are also an excellent candidate for electrical energy storage with high density and reasonable energy efficiency (up to 30% considering storage and fuel cell losses). $Li + H_2O$ and $Na + H_2O$ type storages coupled to a fuel cell are battery-type systems (refilled from electricity and supplying electricity). LiH and NaH type systems, which offer about twice better energy efficiency and storage density, could also be used as battery, provided they are coupled with an electrolyser to supply hydrogen from electricity. In terms of energy density, such systems could compete with existing electrical storage by several orders, at acceptable energy efficiency. However, the practical feasibility of these systems needs to be verified, and the usage should be compatible with the high temperatures of the energy filling electrolytic step.

On long terms, if cycled systems are proven feasible with cycle energy efficiency mostly limited by heat loss on hydrogen release reaction, it may also be worth considering coupling of an endothermal release with the exothermal release, for further heat recycling and improved efficiency.

Finally, for non-chemically-recyclable storage application, where chemicals could be discarded, and where energy cost is not a major issue (storage for small electronics in particular), $\text{AlH}_3 + \text{H}_2\text{O}$, and $\text{NaH} + \text{H}_2\text{O}$ storage offer interesting perspectives. In both cases, the cost of the metal by direct purchase would be $\sim 7\text{eur}$ per kg of H_2 stored (provided low cost production is achieved for sodium). Aluminium potentially offers a far higher storage density than sodium, but the metal should probably be recycled in terms, due to limited world resources.

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US6497973 B1, Engine cycle and fuels for same US6250078 B1, *Fuel blends for hydrogen generators WO2005065119 A2, High energy density boride batteries WO0019553 A1, Hydrogen gas generation system WO2004071946 A2, Hydrogen generator WO2004041714 A2, Method and apparatus for processing discharged fuel solution from a hydrogen WO2004007354 A1, Method and system for generating hydrogen WO2003084866 A2, Portable hydrogen generator WO2003004145 A1, Process for making a hydrogen generation catalyst US6683025 B2, Processes for synthesizing alkali metal borohydride compounds WO2003051957 A1, Processes for synthesizing borohydride compounds WO2002083551 A1, Recycle of discharged sodium borate fuel US6706909 B1, Self regulating hydrogen generator US6939529 B2, System for hydrogen generation WO0151410 A1, Systems and methods for hydrogen generation from solid hydrides WO2005102914 A2, Triborohydride salts as hydrogen storage materials and preparation thereof WO2005065118 A2*

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Annex: How much water can be recycled from a fuel cell?

Knowing that water carried through a fuel cell system is proportional to water partial pressure, noting VP1 vapor pressure in the fuel cell, VP0 outside, VP2 in a cool condenser on FC output, x water humidity outside (humidity in the cell and in the condenser is considered 100%)

Collectable ratio (CR) is $(VP1-VP2)/(VP1-xVP0)$

Ideal ratio

We can hope to have a condenser at ambient temperature at FC exit, so $VP2=VP0$

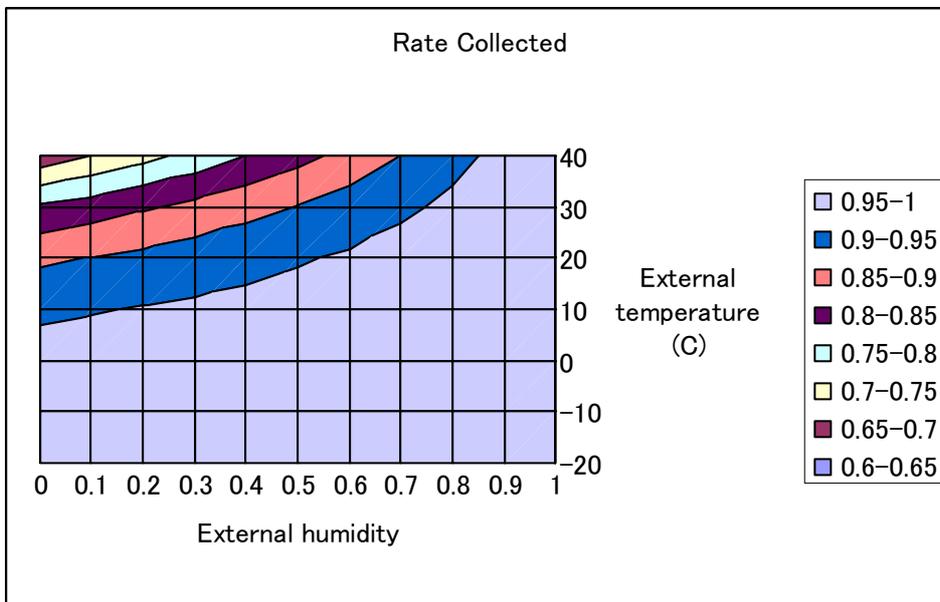
$VP0/VP1$ being small, it follows:

$$CR \sim 1-(1-x)VP0/VP1$$

Rankine formula gives $VP=\exp(a-b/T)$, with $a=13.7$ and $b=5120$, VP in bars, T in K

Hence, $CR \sim 1-(1-x)\exp(b(1/T1-1/T0))$

With Fuel cell temperature (Axane case) $T1\sim 62.5C$:



Ratio with condenser at 40C (Temperature of the humidified in case of axane FC)

Data and reference index

Mass, melting point, density of selected compounds								
	mass (Amu)	ref	Melting point (C)	conditions	ref	dens. (g/ml)	conditions	ref
H	1.008	sargent-welch scientific company						
B (amorp)	10.810	sargent-welch scientific company	2,300.000		chem phys handb	2.370		chem phys handb
N	14.007	sargent-welch scientific company						
O	15.999	sargent-welch scientific company						
Na	22.990	sargent-welch scientific company	97.810		chem phys handb	0.970		chem phys handb
Li	6.941	sargent-welch scientific company	180.540		chem phys handb	0.534	20C	chem phys handb
H2	2.016							
H2Oliq	18.015							
			100.000			1.000		
LiH	7.949							
LiOH	23.948							
			680.000		chem phys handb	0.820		chem phys handb
			450.000		chem phys handb	1.460	!!! Merck gives 2.54!	chem phys handb
Li2O	29.881							
Li2O2	45.881							
NaH	23.998							
			>1700		chem phys handb	2.013	25.2C	chem phys handb
			195.000	dec to Li2O				
			425.000	dec, chem phys hand gives a value of 800C!	Merck	1.396	!!!CPH gives 0.92	Merck
NaOH	39.997							
Na2O	61.979							
			318.400		chem phys handb	2.130		chem phys handb
			1,275.000	sub	chem phys handb	2.270		chem phys handb
Na2O2	77.978							
NaBH4	37.831							
NaBO2	65.799							
Na2B4O7 (crys)	201.215							
			460.000	dec	chem phys handb	2.805		chem phys handb
			400.000	dec	chem phys handb	1.074		chem phys handb
			966.000		chem phys handb	2.464		chem phys handb
			741.000		chem phys handb	2.367		chem phys handb
BHO2 (monocil)	43.817							
BH3O3 (crys)	61.832							
BO2 (gas)	42.809							
B2O3 (crys)	69.618							
Li3N	34.830							
			45.000	trans to glass in N2	chem phys handb	2.460		chem phys handb
			840-850		chem phys handb	1.300		http://www.espimetals.com/msds/lithiumni tride.pdf
Li2HN								
			400<->800	deduced from neighbours				
LiH2N (cryst)								
NH3(g)	17.030							
			380-400		chem phys handb	1.178		chem phys handb
			-77.700	boil -33.5		0.600	at 300K under pressure	http://www.engineerin gtoolbox.com/ammon ia-d_971.html
Mg	24.305	sargent-welch scientific company	648.800		chem phys handb	1.740	5C	chem phys handb
MgH2	26.321							
Mg(OH)2	58.320							
MgO	40.304							
			280.000	diss, vac	chem phys handb	1.450		Merck
			350.000		chem phys handb	2.360		chem phys handb
			2,852.000		chem phys handb	3.580	25C	chem phys handb
Be	9.012	sargent-welch scientific company	1,278.000		chem phys handb	1.850	20C	chem phys handb
BeH2	11.028							
			125.000	dec	chem phys handb	0.637	a verifier	http://www.brushwell man.com/EHS/MSDS /M19.pdf
Be(OH)2	43.027							
BeO	25.012							
			2,530.000		chem phys handb	3.010		Merck
Al	26.982	sargent-welch scientific company	660.370		chem phys handb	2.702		chem phys handb
AlH3 (s)	30.005							
						1.580		http://www.armadilloa erospace.com/n.x/Ar madillo/Home/News? news_id=140
Al(OH)3 (s)	78.003							
Al2O3 (s)	101.961							
			300.000	decomp H2O release	chem phys handb	2.420		chem phys handb
			2,072.000		chem phys handb	3.965	25C	chem phys handb
AlOOH	59.988							
				H2O release, trans to Al2O3	chem phys handb	3.010		chem phys handb
Al2O (gas)	69.962							

Hydrides stabilities and solubilities										
	Enthalpy of formation (kJ/mol) at 298.15K	Entropy standard cond. (J/molK)	Gibbs free energy G=H-TS, (kJ/mol)	Melt (C)	boil	cond / ref	Dec (C)	cond / ref	sol in H2O (g/100 cc) at 100 C	ref cond
H2O (l)	-285.830	69.950	-306.686							
H2O (g)	-241.830	188.726	-298.099							
LiOH (crys)	-484.900	42.800	-497.661	450.000			924	CPHandb	17.5	CPHandb
Li2O (cry)	-597.900	37.600	-609.110							
LiOH -> 1/2Li2O + 1/2H2Oliq	43.035	10.975	39.763							
Li2O2 (cry) peroxide	-634.300	37.600	-645.510							
NaOH (crys)	-425.600	64.500	-444.831	318.4	1390	CPHandb	none		347	CPHandb
Na2O (cry)	-414.200	75.100	-436.591							
NaOH -> 1/2Na2O + 1/2H2Oliq	75.585	8.025	73.192							
Na2O2 (cry) peroxide	-510.900	95.000	-539.224							
Be(OH)2	-902.500	51.900	-917.974	?	?		?			"very slightly

BeO (crys)	-609.400	13.800	-613.514							soluble [®] , mercks
Be(OH)2 -> BeO + H2Oliq	7.270	31.850	-2.226							
Mg(OH)2 (s)	-924.660	63.180	-943.497		none		350		0.004	CPHandb
MgO (s)	-601.600	26.950	-609.635							
Mg(OH)2 -> MgO + H2Oliq	37.230	33.720	27.176							
Al(OH)3 (s)	MISSING DATA!						300		i	CPHandb
Al2O3 (crys)	-1,675.700	50.900	-1,690.876							
Al(OH)3 -> 1/2Al2O3 + 3/2H2O										
Al(OH)3 -> AlOOH + H2O										
Al2O (gas)	-130.000	259.400	-207.340							
AlOOH								to H2O+Al2O3	i	CPHandb

LiOH and LiNH system DATA

	Enthalpy of formation (kJ/mol) 298.15K	of at	ref or Enthalpy step	Entropy standard cond. (J/molK)		Gibbs free energy G=H-TS, (kJ/mol)
H2O (l)	-285.830		CHM	69.950	chem phys handb	-306.686
H2O (g)	-241.830		CHM	188.726	chem phys handb	-298.099
Li (cry)	0.000		chem phys handb	29.100	chem phys handb	-8.676
Na (crys)	0.000		chem phys handb	51.300	chem phys handb	-15.295
H2 (g)	0.000		chem phys handb	130.700	chem phys handb	-38.968
N2(g)	0.000		chem phys handb	191.600	chem phys handb	-57.126
O2 (g)	0.000		chem phys handb	205.000	chem phys handb	-61.121
CO	-110.500		CHM	197.500	chem phys handb	-169.385
CO2	-393.500		CHM	213.676	chem phys handb	-457.207
H2O2 (liq)	-187.800		chem phys handb	109.600	chem phys handb	-220.477

H2 Combustion energy	enthalpie					
H2+1/2O2->H2Oliq	285.830			163.250		237.157
Avogadro	#####	Amu (kg)		0.000		
Energy density MJ/kg	141.795					117.649
Energy density kWh/kg	39.387					32.680

LiOH system

LiH (crys)	-90.500		chem phys handb	20.000	chem phys handb	-96.463
LiOH (crys)	-484.900		chem phys handb	42.800	chem phys handb	-497.661
Li2O (cry)	-597.900		chem phys handb	37.600	chem phys handb	-609.110
Li2O2 (cry) peroxide	-634.300		chem phys handb	37.600	approx = Li2O	-645.510

LiH + H2Oliq + 1/2O2	-376.330	-90.500		192.450		-433.709
Li(OH) + H2 + 1/2O2	-484.900	-108.570		276.000		-567.189
Li(OH) + H2Oliq	-770.730	-285.830		112.750		-804.346
Li + 1/4 O2 + 1/2 H2Ogas + H2Oliq	-406.745	363.985		244.663		-479.691
Li + 1/4O2 +3/2 H2Oliq	-428.745	-22.000		185.275		-483.985
Li + 1/2H2 + 1/2O2 + H2Oliq	-285.830	142.915		266.900		-365.406

1/2Li2O+1/2H2Ogas+H2Oliq	-705.695			183.113		-760.290
1/2Li2O2+1/2H2+H2Oliq	-602.980			154.100		-648.925

Li system

2Li + 2H2Oliq + 1/2O2	-571.660	-44.000		300.600		-661.284
2Li(OH) + H2 + 1/2O2	-969.800	-398.140		318.800		-1,064.850
2Li(OH) + H2Oliq	-1,255.630	-285.830		155.550		-1,302.007
2Li + 1/2 O2 + H2Ogas + H2Oliq	-527.660	727.970		419.376		-652.697

Li2O+H2Ogas+H2Oliq (decomposition a haute T)	-1,125.560			296.276		-1,213.895
Li2O2+H2+H2Oliq	-920.130			238.250		-991.164

NH3 system

NH3(g)	-45.900		NIST/chem phys handb	192.800	NIST/chem phys handb	-103.383
Li3N	-164.560		NIST	62.660	NIST	-183.242
Li2HN	-172.030		deduction des valeurs voisines	62.660	deduction des valeurs voisines	-190.712
LiH2N (cryst)	-179.500		chem phys handbook 5-19	62.660	deduction des valeurs voisines	-198.182

3Li + 1/2N2 + 3H2 + 3/2O2	0.000			882.700		-171.496
NH3(g) + 3LiH + 3/2O2	-317.400			560.300		-392.772
LiNH2 + 2LiH + H2 + 3/2O2	-360.500	-43.100		540.860		-430.076
Li2NH + LiH + 2H2 + 3/2O2	-262.530	97.970		651.560		-365.111
Li3N + 3H2 + 3/2O2	-164.560	97.970		762.260		-300.147
Li3N + 3H2Oliq	-1,022.050	-857.490		272.510		
1/2Li2NH+1/2NH3+2LiH+H2+3/2O2	-289.965			605.930		-378.942
1/2Li2NH+1/2LiNH2+3/2LiH+3/2H2+3/2O2	-311.515			596.210		-397.594

3Li + 1/2N2 + 3/2H2+3/4O2	0.000			532.900		-113.044
NH3(g) + 3Li+3/4O2	-45.900			433.850		-129.412
LiNH2 + 2Li + 1/2H2+3/4O2	-179.500	-133.600		339.960		-235.019
Li2NH + Li + H2+3/4O2	-172.030	7.470		376.210		-238.356
Li3N + 3/2H2 + 3/4O2	-164.560	7.470		412.460		-241.694
Li3N + 3/2H2Oliq	-593.305	-428.745		167.585		
1/2Li2NH+1/2NH3+2Li+1/2H2 +3/4O2	-108.965			405.030		-183.884
1/2Li2NH+1/2LiNH2+3/2Li+3/4H2 +3/4O2	-175.765			358.085		-236.687

NaOH and NaBH4 system DATA

	Enthalpy of formation (kJ/mol) 298.15K	of at	ref or Enthalpy step	Entropy standard cond. (J/molK)		Gibbs free energy G=H-TS, (kJ/mol)
H2O (l)	-285.830		CHM	69.950	chem phys handb	-306.686
H2O (g)	-241.830		CHM	188.726	chem phys handb	-298.099
Li (cry)	0.000		chem phys handb	29.100	chem phys handb	-8.676
Na (crys)	0.000		chem phys handb	51.300	chem phys handb	-15.295
H2 (g)	0.000		chem phys handb	130.700	chem phys handb	-38.968

N2(g)	0.000	chem phys handb	191.600	chem phys handb	-57.126
O2 (g)	0.000	chem phys handb	205.000	chem phys handb	-61.121
CO	-110.500	CHM	197.500	chem phys handb	-169.385
CO2	-393.500	CHM	213.676	chem phys handb	-457.207
H2O2 (liq)	-187.800	chem phys handb	109.600	chem phys handb	-220.477

H2 Combustion energy					
H2+1/2O2->H2Oliq	285.830		163.250		237.157
Avogadro	6.022E+23	Amu (kg)	0.000		
Energy density kJ/kg	1.418E+05				117,649.098
Energy density Wh/kg	39,387.457				32,680.305

NaOH system					
NaH (crys)	-56.300	chem phys handb	40.000	chem phys handb	-68.226
NaOH (crys)	-425.600	chem phys handb	64.500	chem phys handb	-444.831
Na2O (cry)	-414.200	chem phys handb	75.100	chem phys handb	-436.591
Na2O2 (cry) peroxide	-510.900	chem phys handb	95.000	approx = Na2O	-539.224

NaH + H2ONaq + 1/2O2	-342.130	-56.300	212.450		-405.472
Na(OH) + H2 + 1/2O2	-425.600	-83.470	297.700		-514.359
Na(OH) + H2ONaq	-711.430	-285.830	134.450		-751.516
Na + 1/4 O2 + 1/2 H2Ogas + H2ONaq	-406.745	304.685	266.863		-486.310
Na + 1/4O2 +3/2 H2ONaq	-428.745	-22.000	207.475		-490.604
Na + 1/2H2 + 1/2O2 + H2ONaq	-285.830	142.915	289.100		-372.025

1/2Na2O+1/2H2Ogas+H2ONaq	-613.845		201.863		-674.030
1/2Na2O2+1/2H2+H2ONaq	-541.280		182.800		-595.782

Na system					
2Na + 2H2ONaq + 1/2O2	-571.660	-44.000	345.000		-674.522
2Na(OH) + H2 + 1/2O2	-851.200	-279.540	362.200		-959.190
2Na(OH) + H2ONaq	-1,137.030	-285.830	196.950		-1,196.347
2Na + 1/2 O2 + H2Ogas + H2ONaq	-527.660	609.370	463.776		-665.935

Na2O+H2Ogas+H2ONaq	-941.860		333.776		-1,041.375
Na2O2+H2+H2ONaq	-796.730		295.650		-884.878

NaBH4 system					
NaBH4 (crys)	-188.600	chem phys handb	101.300	chem phys handb	-218.803
NaBO2 (crys)	-977.000	chem phys handb	73.500	chem phys handb	-998.914
Na2B4O7 (crys)	-3,291.100	chem phys handb	189.500	chem phys handb	-3,347.599
BHO2 (monocli)	-794.300	chem phys handb	38.000	chem phys handb	-805.630
BH3O3 (crys)	-1,094.300	chem phys handb	88.800	chem phys handb	-1,120.776
BO2 (gas)	-300.400	chem phys handb	229.600	chem phys handb	-368.855
B2O3 (crys)	-1,273.500	chem phys handb	54.000	chem phys handb	-1,289.600

1/4NaBH4 + 1/2H2Oliq + 1/2O2	-190.065	340.015	162.800		-238.604
H2 + 1/4NaBO2 + 1/2O2	-244.250	-54.185	251.575		-319.257
H2Oliq + 1/4NaBO2	-530.080	-285.830	88.325		-556.414

MgH2 BeH2 and AlH3 system DATA

	Enthalpy of formation (kJ/mol) at 298.15K	ref or Enthalpy step	Entropy standard cond. (J/molK)		Gibbs free energy G=H-TS, (kJ/mol)
H2O (l)	-285.830	CHM	69.950	chem phys handb	-306.686
H2O (g)	-241.830	CHM	188.726	chem phys handb	-298.099
Li (s)	0.000	CHM	29.100	chem phys handb	-8.676
Na (crys)	0.000	chem phys handb	51.300	chem phys handb	-15.295
H2 (g)	0.000	CHM	130.700	chem phys handb	-38.968
N2(g)	0.000	chem phys handb	191.600	chem phys handb	-57.126
O2 (g)	0.000	CHM	205.000	chem phys handb	-61.121
CO	-110.500	CHM	197.500	chem phys handb	-169.385
CO2	-393.500	CHM	213.676	chem phys handb	-457.207
NH3(g)	-45.900	NIST/chem phys handb	192.800	NIST/chem phys handb	-103.383

Mg/H/O family					
Mg (crys)	0.000	chem phys handb	32.700	chem phys handb	-9.750
MgH2 (s)	-76.150	NIST	31.030	NIST	-85.402
Mg(OH)2 (s)	-924.660	NIST	63.180	NIST	-943.497
MgO (s)	-601.600	chem phys handb	26.950	chem phys handb	-609.635

1/2MgH2 + H2Oliq + 1/2O2	-323.905	-38.075	187.965		-379.947
1/2Mg(OH)2+H2+1/2O2	-462.330	-138.425	264.790		-541.277
1/2Mg(OH)2+H2O	-748.160	-285.830	101.540		-778.434
1/2MgO+3/2H2Oliq	-729.545	18.615	118.400		-764.846
1/2Mg+1/4O2+3/2H2O	-428.745	300.800	172.525		-480.183
1/2Mg+1/2H2+1/2O2+H2O	-285.830	142.915	254.150		-361.605

hydrogenisation activated by Ni

Be/H/O family					
Be (crys)	0.000	chem phys handb	9.500	chem phys handb	-2.832
BeH2 (crys)	-76.150	approx =MgH2	31.030	approx =MgH2	-85.402
Be(OH)2	-902.500	chem phys handb	51.900	chem phys handb	-917.974
BeO (crys)	-609.400	chem phys handb	13.800	chem phys handb	-613.514

1/2BeH2 + H2Oliq + 1/2O2	-323.905	-38.075	187.965		-379.947
1/2Be(OH)2+H2+1/2O2	-451.250	-127.345	259.150		-528.516
1/2Be(OH)2+H2O	-737.080	-285.830	95.900		-765.673
1/2BeO+3/2H2Oliq	-733.445	3.635	111.825		-766.786
1/2Be+1/4O2+3/2H2O	-428.745	304.700	160.925		-476.725
1/2Be+1/2H2+1/2O2+H2O	-285.830	142.915	242.550		-358.146

Al/H/O family					
AlH3 (crys)	-46.000	chem phys handb			
Al(OH)3 (s)	MISSING DATA!				
Al2O3 (crys)	-1,675.700	chem phys handb	50.900	chem phys handb	-1,690.876
Al2O (gas)	-130.000	chem phys handb	259.400	chem phys handb	-207.340
Al (crys)	0.000	chem phys handb	28.300	chem phys handb	-8.438
AlOOH					

Energy densities							
Family	Technique	kWh/kg	MJ/kg	kWh/l	MJ/l	kg/l systeme	ref and hypothesis
H2 competitors	Gasoline no tank	1.220E+01	4.392E+01	9.700E+00	3.492E+01	7.951E-01	xtronics.com
	Gasoline 45l tank	8.540E+00	3.074E+01	9.700E+00	3.492E+01		Reservoir suppose 30% du poids total
	Methanol no tank	6.400E+00	2.304E+01	4.600E+00	1.656E+01	7.188E-01	xtronics.com
	Ethanol no tank	7.850E+00	2.826E+01	6.100E+00	2.196E+01	7.771E-01	xtronics.com
	Ethanol 45l tank	5.495E+00	1.978E+01	6.100E+00	2.196E+01		Reservoir suppose 30% du poids total
	Compete to ethanol frontier (H2 double efficiency)	0.000E+00	0.000E+00	3.050E+00	1.098E+01		considering half motor efficiency for ethanol
			2.748E+00	9.891E+00	3.050E+00	1.098E+01	
		2.748E+00	9.891E+00	0.000E+00	0.000E+00		
Liquid H2	Liquid H2 no tank	3.900E+01	1.404E+02	2.600E+00	9.360E+00	6.667E-02	xtronics.com
	Liquid H2+Car Cryotank	7.800E+00	2.808E+01	2.600E+00	9.360E+00	3.333E-01	Supose: tank 80% de la masse
High Press 1,150,350,700bar no tank	1bar no tank	3.900E+01	1.404E+02	2.700E-03	9.720E-03	6.923E-05	xtronics.com
	150bar no tank	3.900E+01	1.404E+02	4.050E-01	1.458E+00	1.038E-02	xtronics.com
	350bar no tank	3.900E+01	1.404E+02	8.505E-01	3.062E+00	2.181E-02	deviation GP 10%
	700bar no tank	3.900E+01	1.404E+02	1.323E+00	4.763E+00	3.392E-02	deviation GP 30%
High Press 1,150,350,700bar CF tank 95%mass	1bar	1.950E+00	7.020E+00	2.700E-03	9.720E-03	1.385E-03	densite massique stockage 5% qqsoit pression, densite volumique 100%
	150bar	1.950E+00	7.020E+00	4.050E-01	1.458E+00	2.077E-01	
	350 bar	1.950E+00	7.020E+00	8.505E-01	3.062E+00	4.362E-01	
	700bar	1.950E+00	7.020E+00	1.323E+00	4.763E+00	6.785E-01	
Metal Hydride CF tank light metal (3.5kg/l) 2% absorb , 50% full	1bar	7.802E-01	2.809E+00	1.366E+00	4.919E+00	1.751E+00	conditions proches d'un article publie par Toyota (mater res soc symp proc 884E 2005)
	150bar	8.007E-01	2.882E+00	1.568E+00	5.643E+00	1.958E+00	
	350 bar	8.189E-01	2.948E+00	1.790E+00	6.445E+00	2.186E+00	
	700bar	8.345E-01	3.004E+00	2.027E+00	7.295E+00	2.428E+00	
(hypothetical) CF tank light filler (3.5kg/l) 5% absorb , 50% full	1bar	1.949E+00	7.017E+00	3.414E+00	1.229E+01	1.751E+00	materiau hypothetique
	150bar	1.847E+00	6.648E+00	3.615E+00	1.301E+01	1.958E+00	
	350 bar	1.755E+00	6.320E+00	3.838E+00	1.382E+01	2.186E+00	
	700bar	1.678E+00	6.039E+00	4.074E+00	1.467E+01	2.428E+00	
(hypothetical) CF tank heavy filler (7kg/l) 2% absorb , 50% full	1bar	7.801E-01	2.808E+00	2.731E+00	9.833E+00	3.501E+00	materiau hypothetique
	150bar	7.909E-01	2.847E+00	2.933E+00	1.056E+01	3.708E+00	
	350 bar	8.016E-01	2.886E+00	3.155E+00	1.136E+01	3.936E+00	
	700bar	8.117E-01	2.922E+00	3.392E+00	1.221E+01	4.178E+00	
	start	2.489E+00	8.961E+00	1.804E+00	6.494E+00	7.247E-01	Data de Alldata.xls
	end	1.658E+00	5.966E+00	2.420E+00	8.713E+00	1.460E+00	
LiH+H2O->H2+LiOH	start	9.988E+00	3.596E+01	8.191E+00	2.949E+01	8.200E-01	
	end	3.315E+00	1.194E+01	4.840E+00	1.743E+01	1.460E+00	
2Na+2H2O->H2+2NaOH	start	1.241E+00	4.466E+00	1.214E+00	4.369E+00	9.783E-01	
	end	9.925E-01	3.573E+00	2.114E+00	7.611E+00	2.130E+00	
NaH+H2O->H2+NaOH	start	3.309E+00	1.191E+01	4.619E+00	1.663E+01	1.396E+00	
	end	1.985E+00	7.146E+00	4.228E+00	1.522E+01	2.130E+00	
1/4NaBH4 + 1/2H2Oliq -> H2+1/4NaBO2	start	8.395E+00	3.022E+01	9.016E+00	3.246E+01	1.074E+00	
	end	4.827E+00	1.738E+01	1.189E+01	4.281E+01	2.464E+00	
2Li+2/3NH3(g)->H2+2/3Li3N	start	3.146E+00	1.133E+01	1.768E+00	6.363E+00	5.618E-01	
	end	3.419E+00	1.231E+01	4.445E+00	1.600E+01	1.300E+00	
LiH+1/3NH3(g)->H2+1/3Li3N	start	5.827E+00	2.098E+01	4.145E+00	1.492E+01	7.113E-01	
	end	6.839E+00	2.462E+01	8.890E+00	3.201E+01	1.300E+00	
1/2MgH2 + H2Oliq -> H2+1/2Mg(OH)2	start	6.033E+00	2.172E+01	8.748E+00	3.149E+01	1.450E+00	
	end	2.723E+00	9.802E+00	6.426E+00	2.313E+01	2.360E+00	
1/2BeH2 + H2Oliq -> H2+1/2Be(OH)2	start	1.440E+01	5.184E+01	9.167E+00	3.300E+01	6.366E-01	
	end	3.691E+00	1.329E+01	7.086E+00	2.551E+01	1.920E+00	
1/3AlH3 + H2O -> 1/3Al(OH)3 + H2	start	7.938E+00	2.858E+01	1.254E+01	4.515E+01	1.580E+00	
	end	3.054E+00	1.099E+01	7.390E+00	2.660E+01	2.420E+00	

Energy Efficiency Comparison												
	Li H2O +	LiH H2O non h recycl	LiH H2O h recycl	Na H2O +	NaH H2O non h recycl	NaH H2O h recycl	NaBH4 + H2O	Li NH3 +	LiH NH3 +	MgH2 + H2O h recycl	BeH2 + H2O h recycl	AlH3 + H2O h recycl
Effi. on filling	0.940	0.778	1.000	0.928	0.825	1.000	0.000	0.000	0.849	0.000	0.000	
Loss on filling (kJ/mol)	0.060	0.222	0.000	0.072	0.175	0.000	1.000	1.000	0.151	1.000	1.000	
Effi. on release	0.418	0.725	0.725	0.506	0.774	0.774	0.841	1.000	1.000	0.674	0.692	
Loss on release (kJ/mol)	0.547	0.214	0.275	0.459	0.186	0.226	0.000	0.000	0.000	0.000	0.000	
Effi. On FC	0.400	0.400	0.400	0.400	0.400	0.400	0.400	0.400	0.400	0.400	0.400	0.400
Loss on FC	0.236	0.338	0.435	0.281	0.383	0.464	0.000	0.000	0.509	0.000	0.000	
Effi. of e motor	0.950	0.950	0.950	0.950	0.950	0.950	0.950	0.950	0.950	0.950	0.950	0.950
Loss on e motor	0.008	0.011	0.014	0.009	0.013	0.015	0.000	0.000	0.017	0.000	0.000	
Usable energy	0.149	0.214	0.275	0.178	0.243	0.294	0.000	0.000	0.323	0.000	0.000	
Total loss	0.851	0.786	0.725	0.822	0.757	0.706	1.000	1.000	0.677	1.000	1.000	
Effi. fillingXrelease	0.393	0.564	0.725	0.469	0.639	0.774	0.000	0.000	0.849	0.000	0.000	

Element Prices and availabilities		
Li supply	\$/kg	ref
LiOH.H2O cheapest (\$/kg)	2.37	China -> US custom value 2004. NOTE: Price decrease possible in 2006 due to new SQM factory in Chile
Corresponding Li Price (\$/kg)	14.32823945	
LiCO3 cheapest (\$/kg)	1.45	Chile->US custom value 2004
Corresponding Li Price (\$/kg)	13.9858882	
Identified world reserves of Li as ? (kg)	1.300E+10	2006 data, Bolivia, Chile, China are main
Annual production of Li (kg), brine -> LiCO3 mostly	2.000E+07	2006 data, Chile is main

Na supply		ref
NaCO₃ (soda ash) cheapest (\$/kg)	0.11	US->world mean custom value 2004
Corresponding Na Price (\$/kg)	0.397119617	
Identified world reserves of NaCO ₃ (kg)	8.100E+13	2006 data, US is main
Corresponding Na mass (kg)	2.244E+13	
Annual production of NaCO ₃ (kg)	4.030E+10	2006 data, China and US are main
NaOH cheapest (kg/\$)	4.000E-01	From http://www.kasteelchemicals.com/newcaustic.html , fluctuation from 30 to 500 \$/ton!, mostly brine electrolysis
Corresponding Na Price (\$/kg)	0.695902566	
NaCl cheapest (\$/kg)	7.000E-03	2006 data salt in brine
Corresponding Na Price (\$/kg)	0.017794737	
Identified world reserves of NaCl (kg)	inexhaustible	
Annual production of NaCl (kg)	2.100E+11	continental only, 2006 data
Na₂SO₄ (sodium sulfate) cheapest (\$/kg)	1.477E-01	2005 data
Corresponding Na Price (\$/kg)	0.456287475	
Identified world reserves of Na ₂ SO ₄ (kg)	4.6E+12	
Corresponding Na mass (kg)	1.48912E+12	
Mg supply		ref
MgO cheapest (\$/kg)	0.400139024	US mean price 2004
Corresponding Mg Price (\$/kg)	0.663534384	
Mg(OH)₂ cheapest (\$/kg)	8.818E-01	US mean price 2004
Corresponding Mg Price (\$/kg)	2.115965903	
MgCl₂ cheapest (\$/kg)	2.811E-01	US mean price 2004
Corresponding Mg Price (\$/kg)	1.101123209	
Mg as Mg cheapest (\$/kg)	3.858E+00	2004 data
Identified world reserves of Mg as MgCO₃ (kg)	1.200E+13	2006 data for MgCO ₃ (magnesite) only (Mg(OH) ₂ also available from sea)
Be supply		ref
BeO and Be(OH)₂ cheapest (\$/kg)	11.32	US custom import price 2004
Corresponding Be Price (\$/kg)	54.04405306	assumed Be(OH) ₂
Be unwrought cheapest (\$/kg)	1.400E+02	US custom import price 2004
Identified world reserves of Be (kg)	8.000E+07	2005 data
Annual production of Be (kg)	1.120E+05	2004 data
Al supply		ref
Al₂O₃ cheapest (\$/kg)	0.371	US custom import price 2004
Corresponding Al Price (\$/kg)	0.700982777	
Identified world reserves of Al ₂ O ₃ (kg)	1.190E+09	aluminium oxide 2005 data
Corresponding Al mass (kg)	6.298E+08	
Al cheapest (\$/kg)	1.940E+00	US custom import price 2004
Identified world reserves of Al (kg)	3.550E+10	2005 data
B supply		ref
Na₂B₄O₇·5H₂O (borax pentahydrate) cheapest (\$/kg)	0.4	US price 2005
Corresponding B Price (\$/kg)	2.694616096	
Identified world reserves (kg)	4.100E+11	2005 data
NaBH ₄ cheapest	12	Estimation K. Barral AL ref 238-2004. Hypothetical minimal price.

Table of contents

Page	
2	Abstract
3	1. Introduction
5	2. How we select the reactions
5	2.1. Available reactions
6	2.2. Release reactions with water
6	2.2.1. Reactions of elements with water
8	2.2.2. Reactions of diatomic hydrides with water
9	2.3. Recycling by melted salt electrolysis
11	3. Li/O/H based systems
11	3.1. Generalities
12	3.2. Reaction pathway
13	3.3. Efficiency
16	3.4. Storage densities
16	3.5. Technical feasibility
18	4. Na/O/H based systems
18	4.1. Generalities
18	4.2. Reaction pathway
19	4.3. Energy Efficiency
20	4.4. Storage densities
20	4.5. Technical feasibility
20	5. Na/B/O/H based systems (NaBH₄)
20	5.1. Generalities
21	5.2. Reaction pathway
22	5.3. Storage densities
22	6. Higher hydrides (MH₂, MH₃)
22	6.1. Mg/O/H based systems
24	6.2. Be/O/H based systems
25	6.3. Al/O/H based systems
25	7. Li/N/H based systems
25	7.1. Generalities
26	7.2. Reaction pathways
28	7.3. Storage densities
28	7.4. Technical feasibility
30	8. Comparison
30	8.1. Energy density
31	8.2. Storage efficiency
33	8.3. Element prices and availabilities
36	9. Conclusions
38	Related Bibliography
41	Annex: How much water can be recycled from a fuel cell?
42	Data and reference index