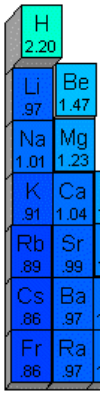
Hydrogen – General

- Colorless, odorless, non toxic and highly flammable diatomic gas.
- Most abundant element in the universe.
- Fuel of the sun.
- Jupiter: 99.8 % hydrogen and helium.

Jupiter

Despite its position on top of Group I, it is not really part of this group:

- It is a gas and not a metal.
- No reaction with water.
- Far more electronegative than the alkali metals.



Electronegativity of Group I and II

Hydrogen – History

- 1766: Discovered and isolated by Henry Cavendish.
- 1781: Cavendish demonstrated that when hydrogen burned it formed water, thereby disproving the Aristotelian theory of four elements of which water was one.
- 1898: James Dewar produced the first liquid hydrogen.
- 1900: the first ‘Zeppelin’ made its flight filled with hydrogen.
- 1931: Harold Urey discovered deuterium.

Henry Cavendish (1731-1810)

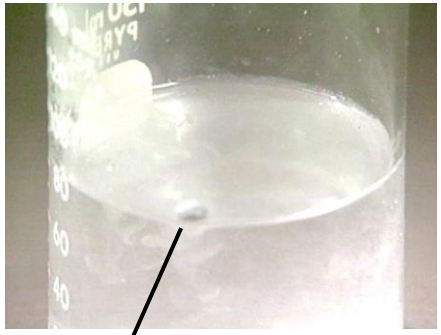
Hindenburg fire in 1937

Synthesis of Hydrogen

Electropositive metals react with water to give hydrogen:

$2\ Na + 2\ H_2O \longrightarrow H_2 + 2\ Na^+ + 2\ OH^-$

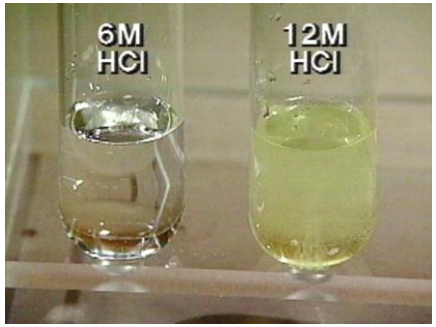
$Ca + 2\ H_2O \longrightarrow H_2 + Ca^{2+} + 2\ OH^-$



Piece of Na in H_2O

In the lab: reaction of Fe or Zn with acids:

$Zn + 2\ H_3O^+ \longrightarrow H_2 + Zn^{2+} + 2\ H_2O$

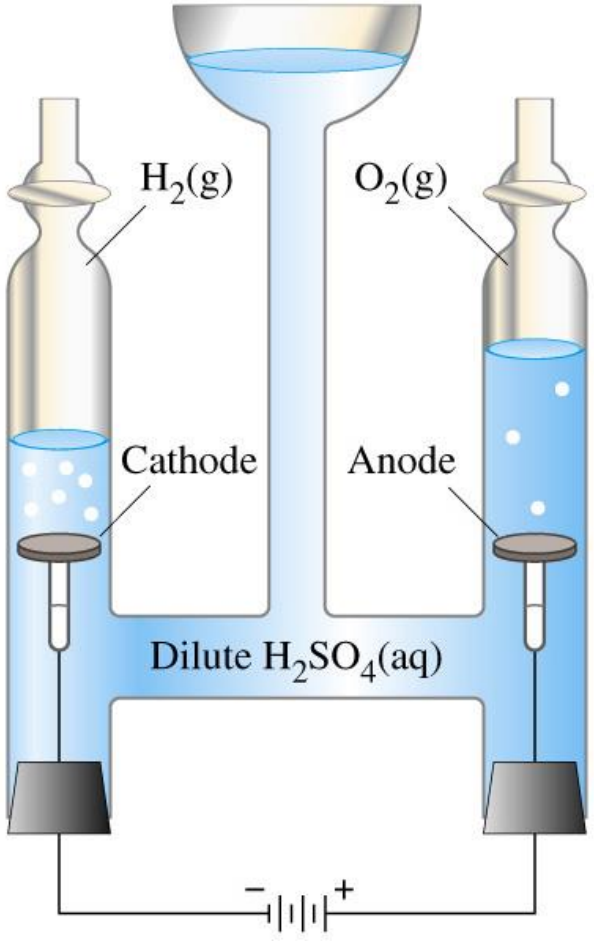


Pieces of Fe in HCl/H_2O

Synthesis of Hydrogen

Electrolysis of water

- By electrolysis of H_2SO_4 or KOH.
- Produces very clean hydrogen.



Technical Production of Hydrogen

- Most hydrogen is produced from natural gas (mainly methane).
- Half of the produced hydrogen is uses for the synthesis of NH_3.

Steam reforming

$$CH_4 + H_2O \xrightarrow[800\ °C]{[Cat.]} 3\ H_2 + CO$$

Synthesis gas
'Syngas'

Steam reforming plant
at BASF

Uses of syngas:

$$m\ CO(g) + n\ H_2(g) \xrightarrow{[Cat.]} \text{'CH' or 'CHO' products}$$

'CH' = gasoline, waxes; 'CHO' = methanol, glycols

Technical Production of Hydrogen

Coal gasification

$$C + H_2O(g) \xrightarrow{\sim 1000\ ^\circ C} H_2 + CO$$

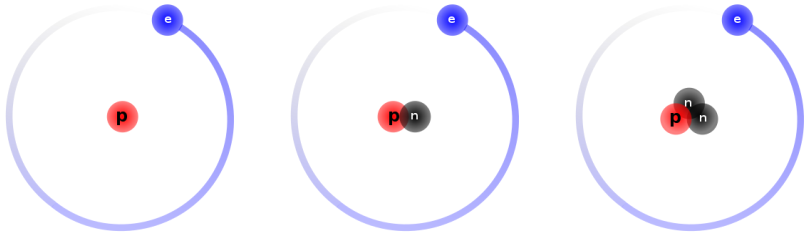
Since coal gasification is an endothermic process energy is required, which is obtained by the burning of coal. The CO generated by steam reforming or coal gasification can be converted in the **water-gas shift reaction**:

$$CO + H_2O \longrightarrow H_2 + CO_2$$

2544-ton-per-day coal gasification demonstration pilot plant

Hydrogen – Isotopes

	nucleus	*abundance*	
^{1}H	1 proton	99.985 %	
^{2}H (D)	1 proton, 1 neutron	0.015 %	
^{3}H (T)	1 proton, 2 neutrons	10^{-15} %	(radioactive)



$^{1}_{1}H$ $^{2}_{1}H$ $^{3}_{1}H$

Protium Deuterium Tritium

Deuterium

- For no other element the relative mass differences are so big. This results in pronounced differences in chemical reactivity.
- H_2 is more reactive than D_2. Electrolysis of H_2O leads to an enrichment of D_2O.
- Isotope effects can be useful to probe the mechanism of a reaction.
- Deuterated compounds can be obtained in exchange reactions:

$$SiCl_4 + 2\ D_2O \longrightarrow SiO_2 + 4\ DCl$$

- D_2O is used in nuclear reactors as a moderator because it can slow down neutrons.
- Deuterated compounds are extensively used in Nuclear Magnetic Resonance experiments (NMR).

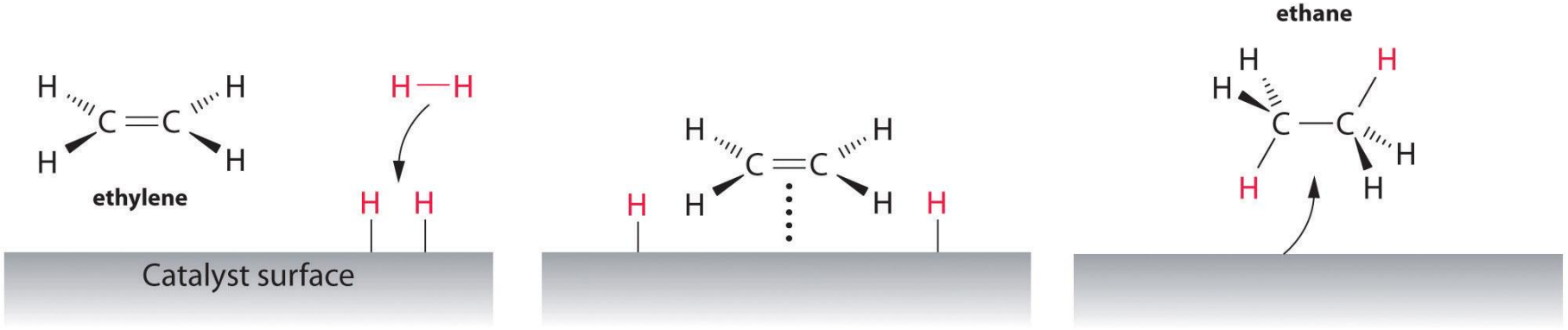
Heavy Water Ice Cubes

An ice cube made from normal water floats in a beaker of liquid water.

An ice cube of deuterium oxide sinks in water.

Reactivity of Hydrogen

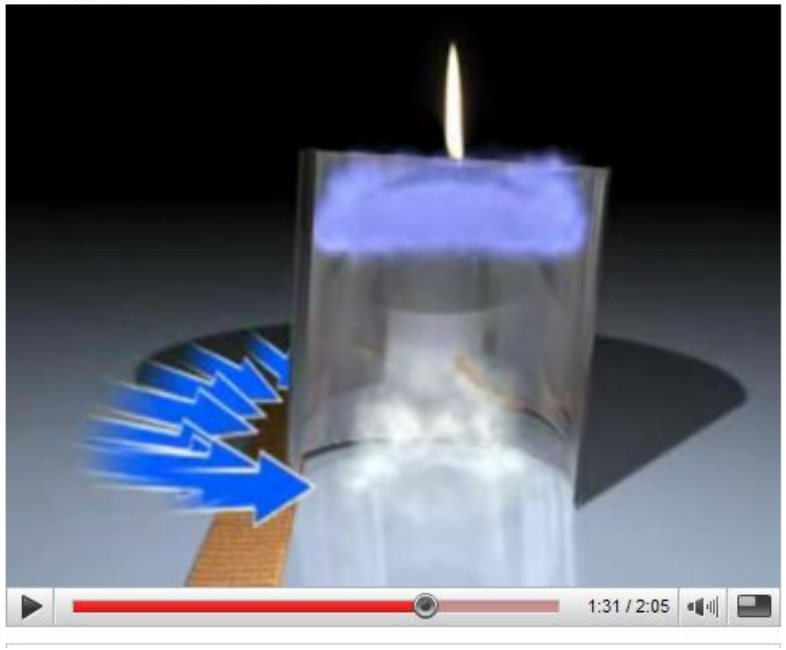
- At room temperature, H_2 is not very reactive due to the high dissociation energy.
- H_2 can be activated on the surface of catalysts.

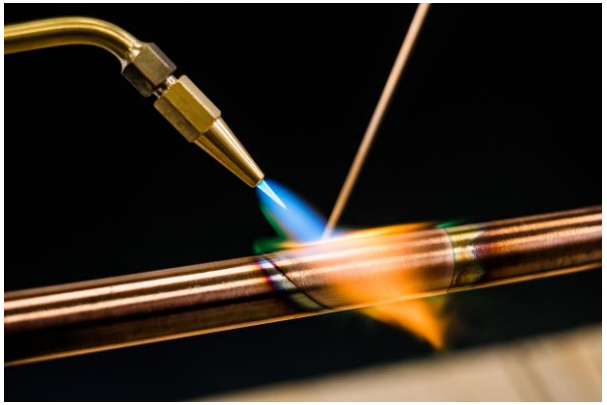


Hydrogen – Reaction with O_2

$$H_2 + 1/2\ O_2 \longrightarrow H_2O(g) \qquad \Delta H° = -242\ kJ/mol$$

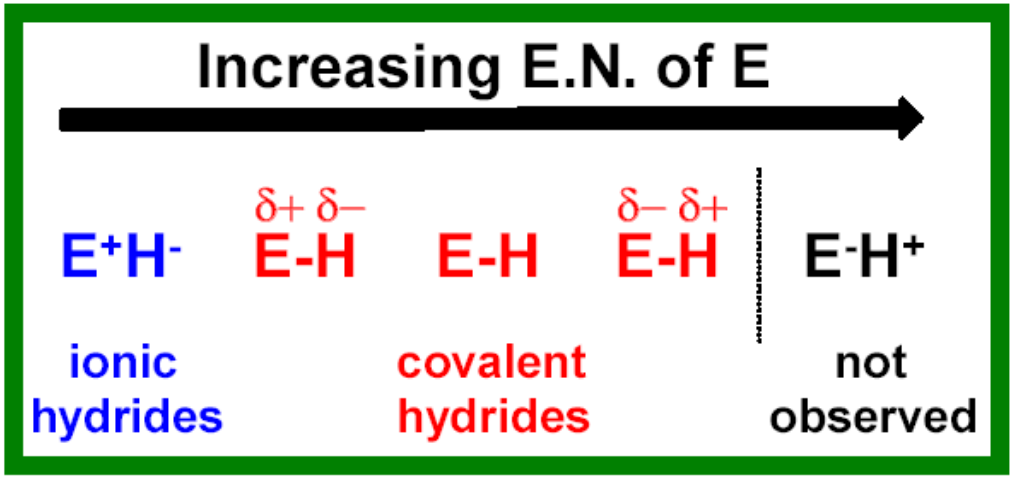
Knallgas - GALILEO





http://www.youtube.com/watch?v=vRx34APjmQU

Hydrogen in Compounds



H is of intermediate electronegativity (2.1)

Ionic Hydrides

- H^- forms with extremely electropositive elements (Group I, heavier Group II) and it behaves much like Cl^- as might be expected on the basis of size and charge:

	radius (r)	Q/r ratio
H	0.32 Å	
H^-	1.53	0.65
F^-	1.19	0.84
Cl^-	1.67	0.60

- Evidence for true H^-:
  a) conduct electricity in the melt like NaCl
  b) electrolysis results in $H_2(g)$ at the anode (+).

$$NaH(l) \xrightarrow[\text{in melt}]{\text{electrolysis}} \underset{\text{cathode}}{Na(l)} + \underset{\text{anode}}{1/2\ H_2(g)}$$

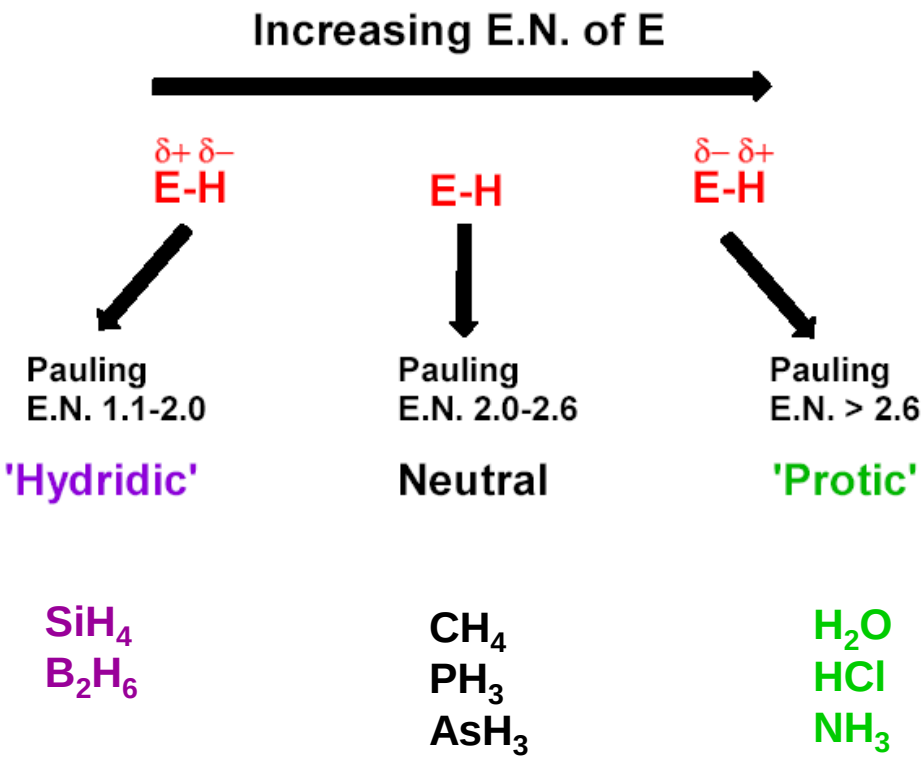
- Ionic hydrides react with water:

drying agent

$$CaH_2(s) + H_2O(l) \longrightarrow Ca(OH)_2 + H_2(g)$$

$$H^- + H^+ \longrightarrow H_2(g)$$

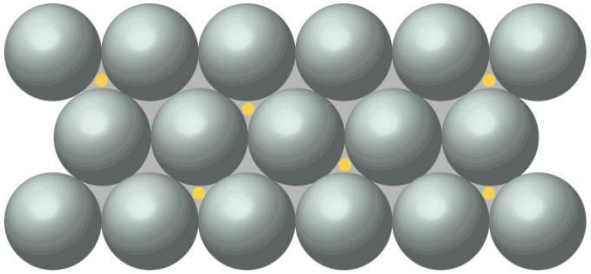
Covalent Hydrides



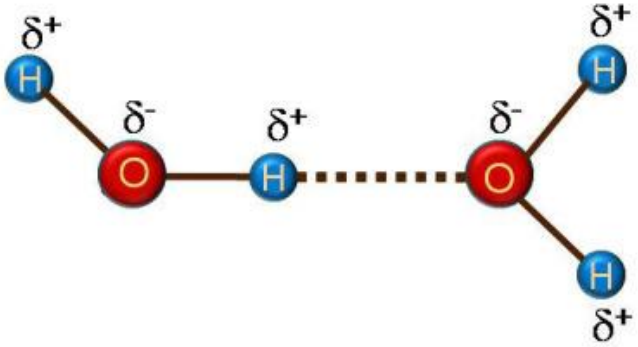
Metallic Hydrides

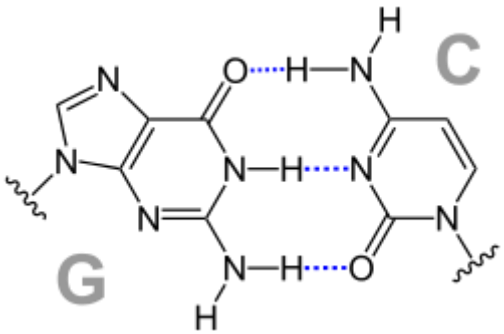
Some transition metals and alloys form nonstoichiometric hydrides in which the hydrogen atoms sit in the octahedral and tetrahedral voids of the metal lattice (‘interstitial hydrides’). Conducting or semi-conducting solids with metallic look.

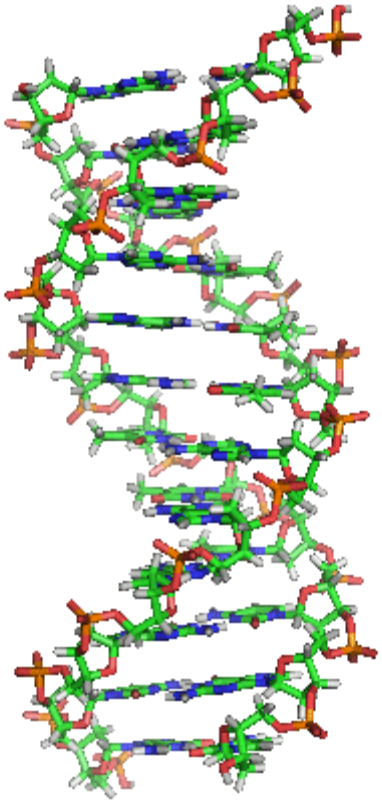
e.g. $TiH_{1.9}$ $HfH_{2.1}$



Hydrogen Bonds







Hydrogen as a Fuel

The Hydrogen Fuel Cell car from Hyundai

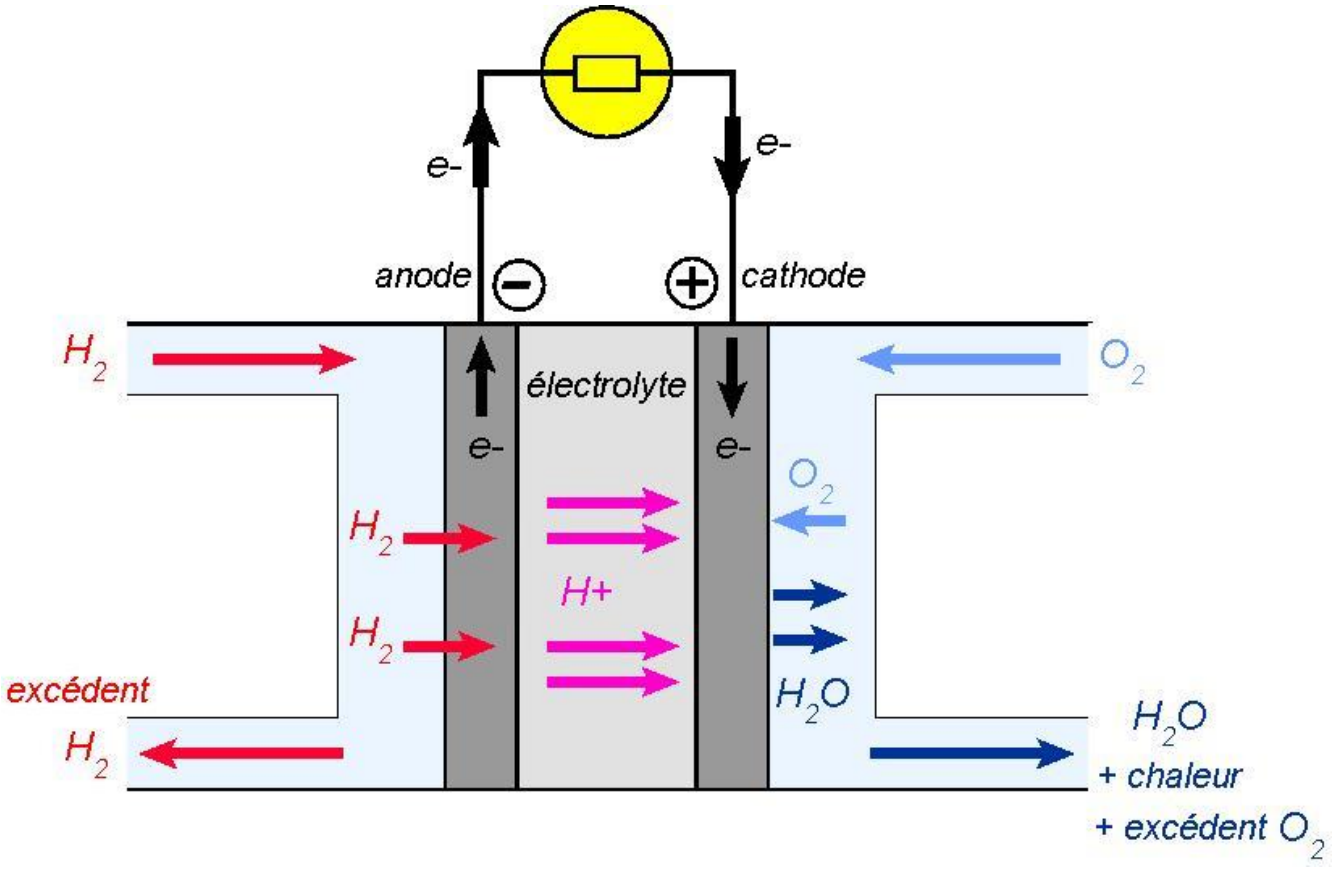
Space shuttle: 500 000 l of liquid O_2 and 1.5 million liters of liquid H_2

Hydrogen is either burned or converted into electricity in a fuel cell.

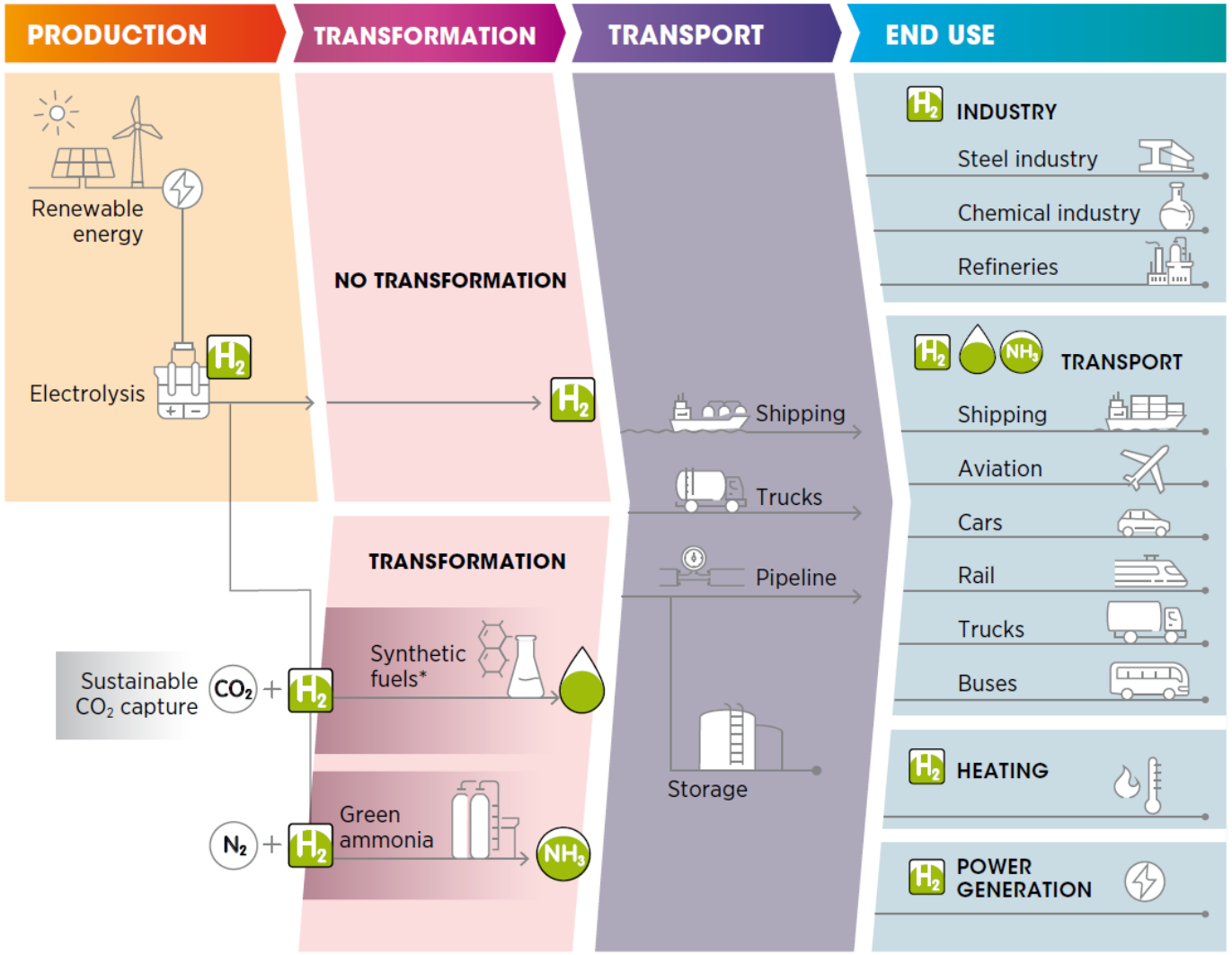
Hydrogen as a Fuel

2035 ?

Fuel Cell Technology



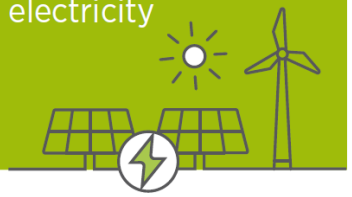
Hydrogen Economy



IRENA
International Renewable Energy Agency

The Colors of Hydrogen

Color	GREY HYDROGEN	BLUE HYDROGEN	TURQUOISE HYDROGEN*	GREEN HYDROGEN
Process	SMR or gasification	SMR or gasification with carbon capture (85-95%)	Pyrolysis	Electrolysis
Source	Methane or coal	Methane or coal	Methane	Renewable electricity



(pilot phase)

Note: SMR = steam methane reforming.
** Turquoise hydrogen is an emerging decarbonisation option.*

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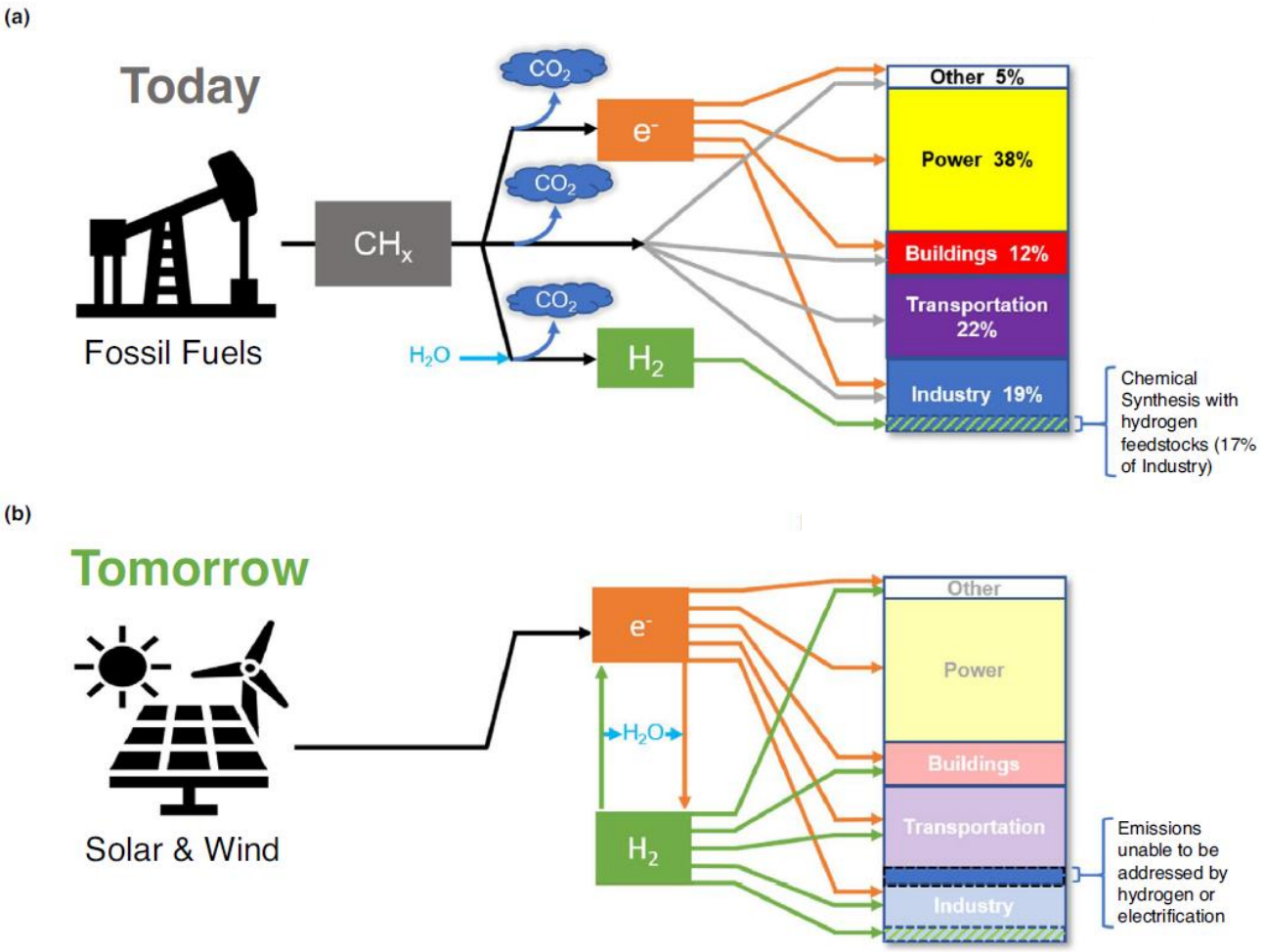
Hydrogen Economy



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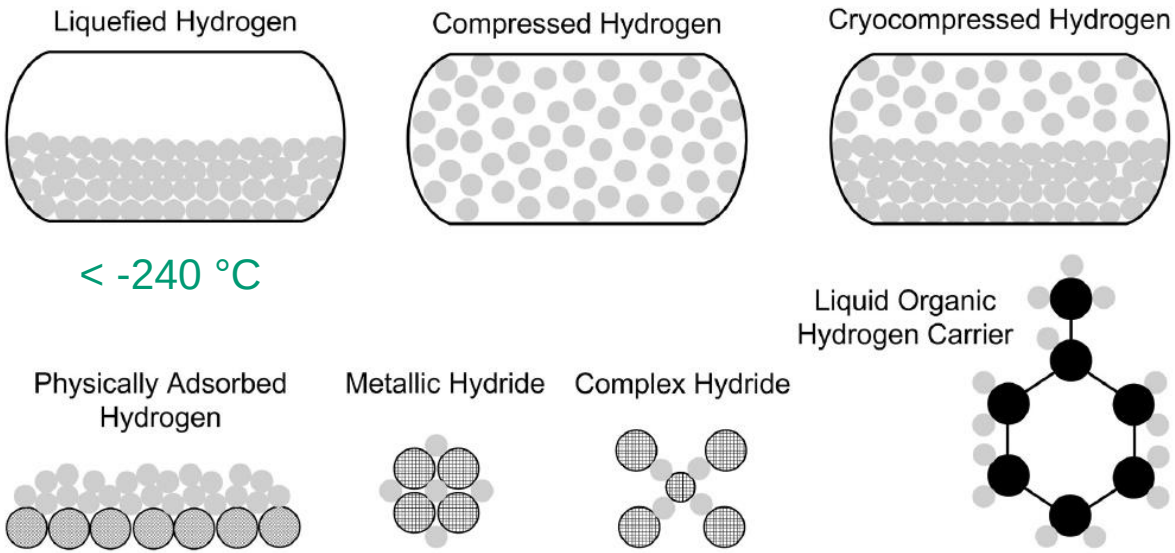
Hydrogen Storage



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