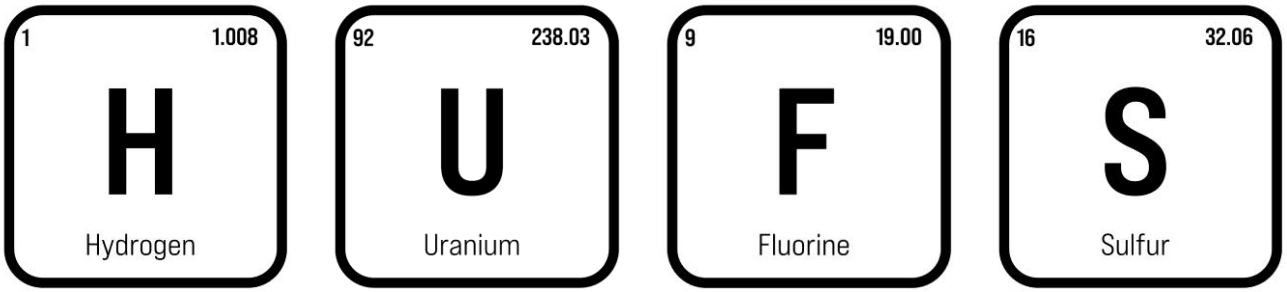
01st Sep 2026



수소경제와 에너지저장 시스템

(Hydrogen Economy and Energy Storage Systems)

Haewon Seo, Ph. D

Hydrogen **E**nerg**Y** Lab **ON E**arth

Assistant Professor

Division of Climate Change

Hankuk University of Foreign Studies (HUFS)

Course Introduction

- **Lecture: Hydrogen Economy and Energy Storage Systems (L01212101)**
  - Class time: Tuesday, 15:00–17:50

- **Professor**: Haewon Seo
  - Office: Prof Res Bldg , Rm 202
  - E–mail: heyone@hufs.ac.kr
  - Office hour: Monday (till 15:00)

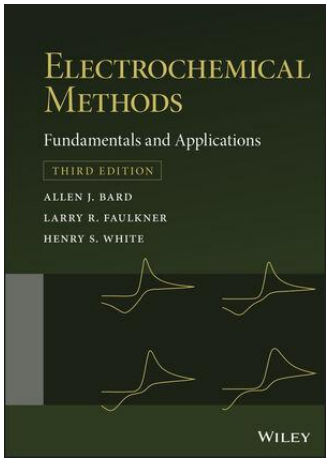
- **Scope**
  - This course introduces hydrogen energy and its associated devices for a clean and sustainable future. Based on fundamental electrochemistry, it examines the operating principles of energy conversion systems for hydrogen production and utilization. Furthermore, it reviews the latest technological trends and explores the development of next-generation energy conversion technologies.

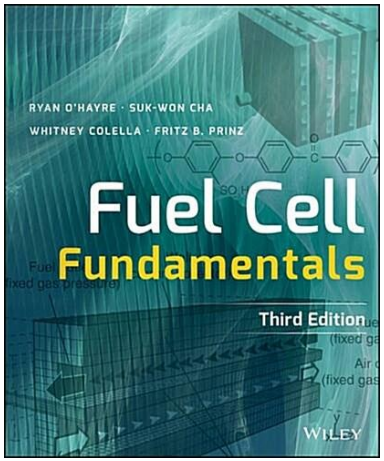
Course Introduction

❑ Textbook

– Main

- Electrochemical Methods (A.J. Bard et al.), 3rd Ed., Wiley (2022)
- Thermodynamics (Y.A. Cengel et al.), 9th Ed., McGraw-Hill (2018)
- Fuel Cell Fundamentals (R. O'Hayer et al.), 3rd Ed., Wiley (2016)





– Reference

- Scientific articles
- IRENA, IEA, World Energy Council, DOE, etc.

Course Introduction

- **Schedule**; to be flexibly operated

Week	Date	Contents
01st	**Sep 01st 2026**	**Introduction to Hydrogen (1)**
02nd	Sep 08th 2026	Introduction to Hydrogen (2)
03rd	Sep 15th 2026	Laws of Thermodynamics (1)
04th	Sep 22nd 2026	Laws of Thermodynamics (2)
05th	Sep 29th 2026	Thermodynamics of Reacting Systems
06th	Oct 06th 2026	Electrochemical Cells & Potentials
07th	Oct 13th 2026	Reference Electrodes & Practical Cells
08th	Oct 20th 2026	Midterm exam
09th	Oct 27th 2026	Cell Polarization & Overpotentials
10th	Nov 03rd 2026	Electrode Kinetics & Interface (EDL)
11th	Nov 10th 2026	Mass Transport & Chronoamperometry
12th	Nov 17th 2026	Voltammetry & Reaction Mechanisms
13th	Nov 24th 2026	Electrochemical Impedance
14th	Dec 01st 2026	Applications
15th	Dec 15th 2026	Final exam

Course Introduction

- **Evaluation**
  - Attendance (10%)
  - Assignment (20%)
  - Midterm Exam (30%)
  - Final Exam (40%)

1. Introduction to Hydrogen (1)

Contents

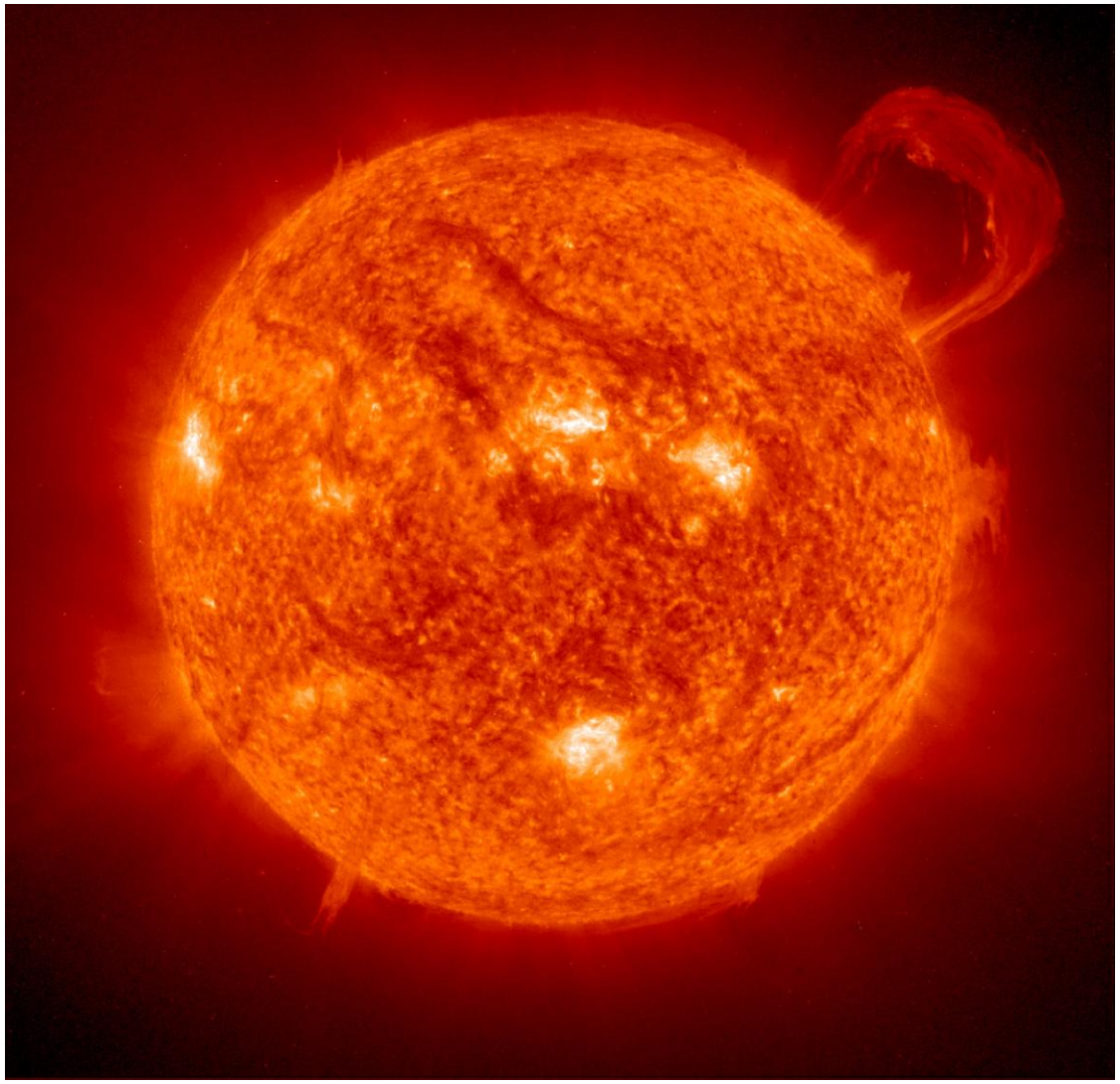
1. Overview of Hydrogen

2. Necessity of Hydrogen

3. Basic of Thermodynamics

4. Hydrogen Production Technology

Overview of Hydrogen

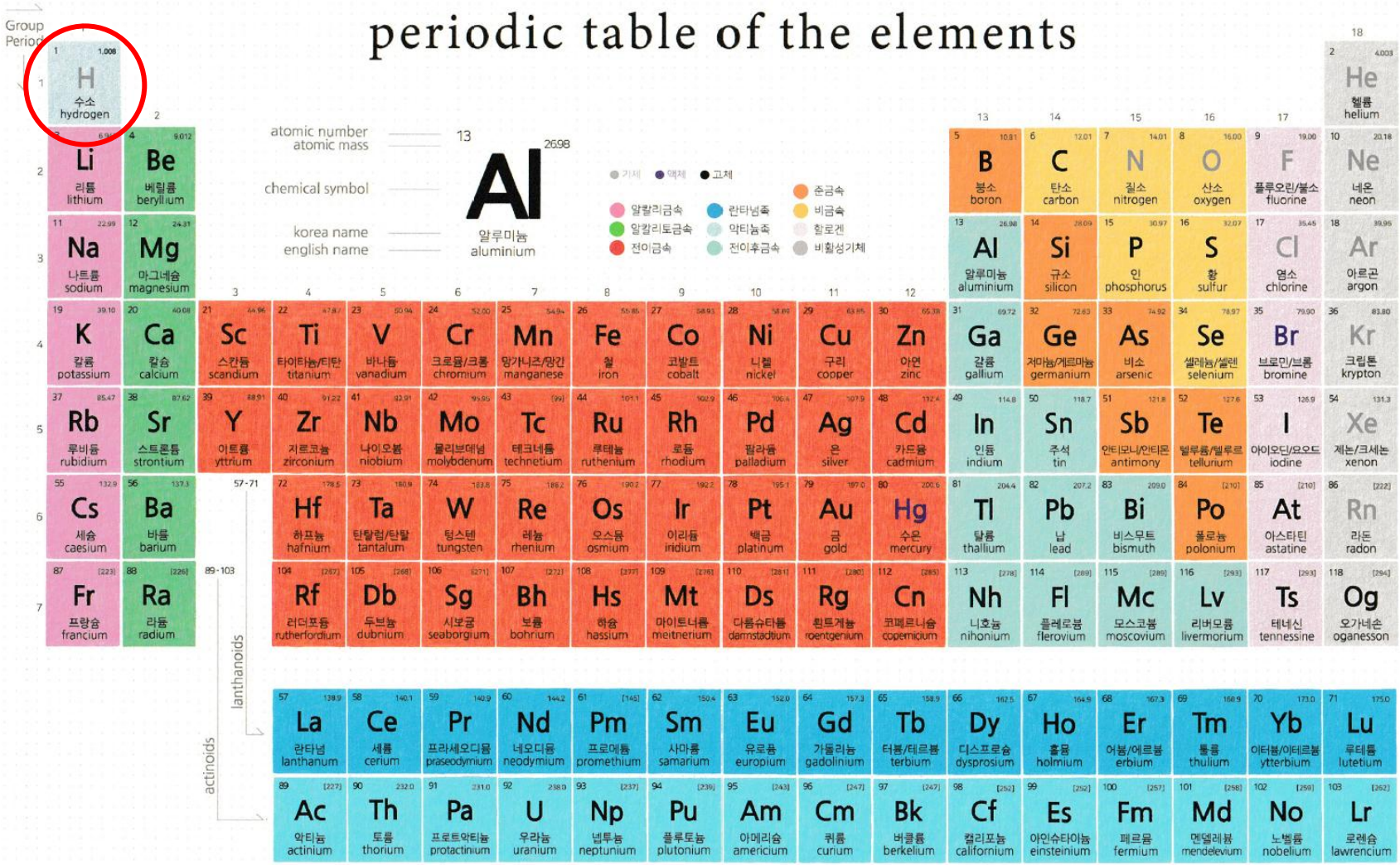


<Source: NASA>

Overview of Hydrogen

❑ Hydrogen

The simplest element in the universe (one proton, one electron, and no neutron)



Overview of Hydrogen

❑ Hydrogen

The simplest (one proton & one electron) and abundant (~75%) element in the universe

- Symbol: H
- Atomic Number: 1
- Atomic Weight: 1.0079 u
- Melting Point: –259.2 °C
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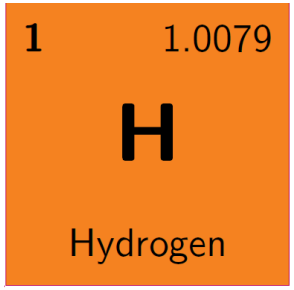
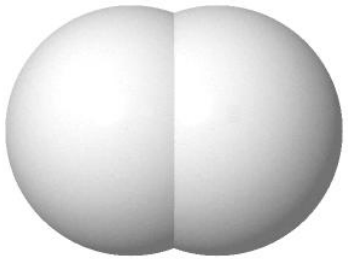
- Density: 0.090 g L^{-1} (at STP (0 °C, 1 atm))





–Typically, hydrogen refers to *hydrogen gas* (H_2), which is a colorless, odorless, and nontoxic gas

Table Physical properties of gases at standard temperature and pressure (STP) (0 °C, 1 atm)

Gas	Density, ρ (g L^{-1})	Specific heat capacity, C_p (J g^{-1} K^{-1})	Thermal cond., k (W m^{-1} K^{-1})	Viscosity, μ (μPa s)
H_2	**0.090**	**14.28**	**0.168**	**8.4**
He	0.179	5.19	0.142	18.6
CH_4	0.717	2.22	0.030	10.3
Air	1.292	1.005	0.024	17.2
O_2	1.429	0.915	0.024	19.2
CO_2	1.977	0.823	0.015	13.7

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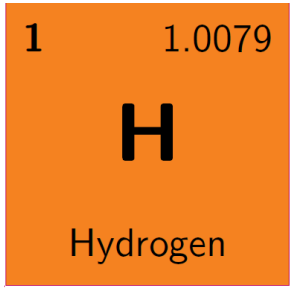

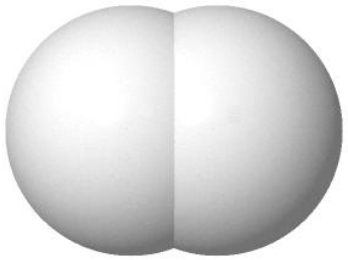

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Table Physical properties of liquids

Liquid	Density, ρ (g L^{-1})	Boiling point (°C)	Remarks
H_2	**70.85**	**–252.9**	**~1/6 of CH4's density**
He	125.0	–268.9	
CH_4	422.8	–161.5	
Air	874.0	–194.3	
O_2	1141	–183.0	
CO_2	1178	–78.5	At triple–point

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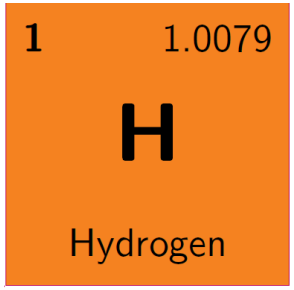

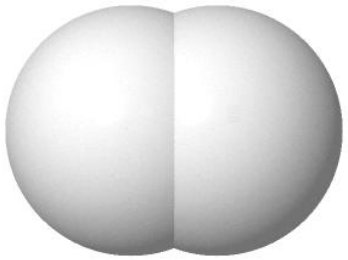

–H_2 makes up ~0.5–0.6 ppm of the Earth's atmosphere, whereas H is ubiquitous in water (H_2O), organic compounds (CHONPS), and other matter.

Table Major constituents of the atmosphere of Earth in parts–per million (ppm)

Gas	Volume fraction (ppm)	Gas	Volume fraction (ppm)	Gas	Volume fraction (ppm)
N_2	780,840	CH_4	1.92	O_3	0.07
O_2	209,460	Kr	1.14	NO_2	0.02
Ar	9,340	**H_2**	**0.55**	H_2O	Up to 40,000
CO_2	420	N_2O	0.33		
Ne	18.182	CO	0.10		
He	5.24	Xe	0.09		

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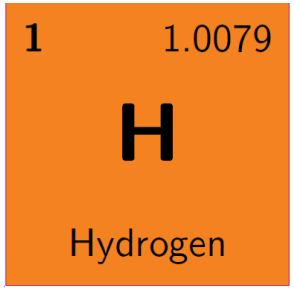
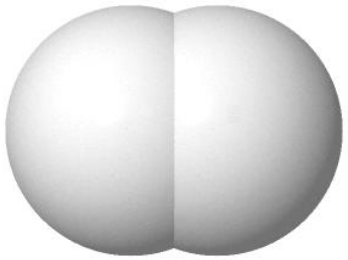
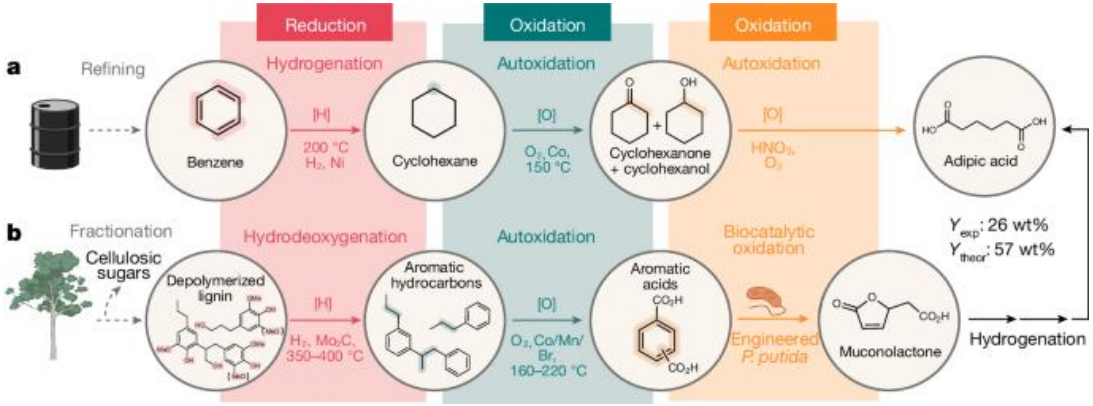




*$H_2 \rightarrow 2H$ ($\Delta H° = 435.14$ kJ mol^{-1})

–Low reactivity at room temperature, but reacts with most elements and compounds at high temperatures or in the presence of catalysts

–Involved in biological redox (oxidation–reduction) reactions



Nature, **654** (2026) 668–675

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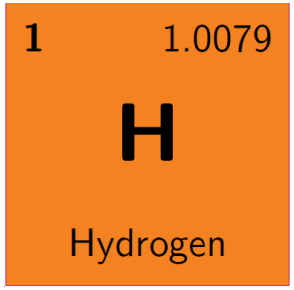
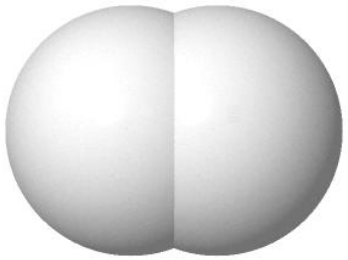




–Reacts with halogens to form hydrogen halides, and with CO to produce hydrocarbons and alcohols

*$H_2 + X_2 \rightarrow 2HX$ (X = F, Cl, Br, I)

**$nCO + (2n+1)H_2 \rightarrow C_nH_{2n+2} + nH_2O$

***$nCO + 2nH_2 \rightarrow C_nH_{2n+1}OH + (n-1)H_2O$

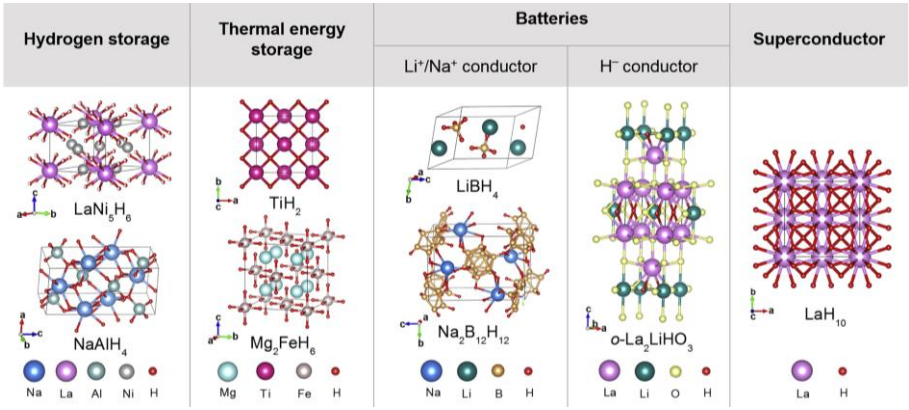
–Combines with numerous elements to form various hydrides

*Ionic hydride (groups 1, 2 except for Be, Mg) (e.g., LiH, NaH, CaH_2, etc.)

**Covalent hydride (groups 13–17) (e.g., B_2H_6, CH_4, NH_3, H_2O, HF, etc.)

***Metallic hydride (typically transition metals) (e.g., TiH_2, PdH_x, etc.)

***Complex hydride (e.g., $NaBH_4$, $LiAlH_4$, $NaAlH_4$, etc.)



Joule, **4**(4) (2020) 705–709

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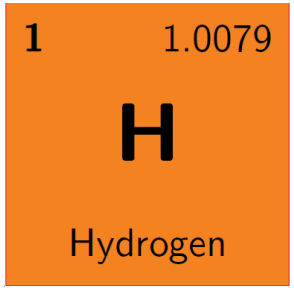
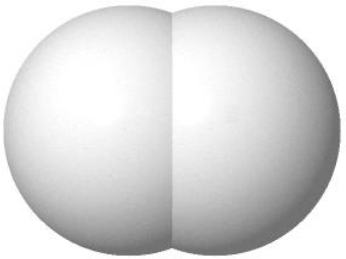
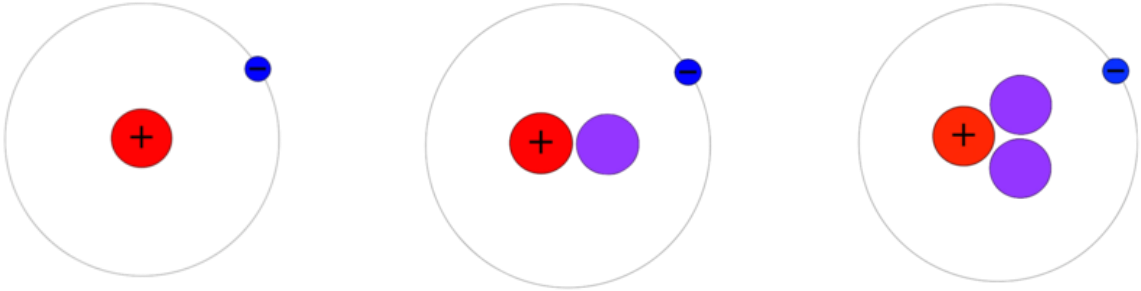




–Hydrogen has three main naturally occurring isotopes: ^{1}H (protium), ^{2}H (D) (deuterium), ^{3}H (T) (tritium)



	Protium	Deuterium	Tritium
Atomic Weight	1.0079 u	2.0141 u	3.0160 u
Half-Year	Stable	Stable	12.32 yr
Abundance	99.9855%	0.0115%	trace

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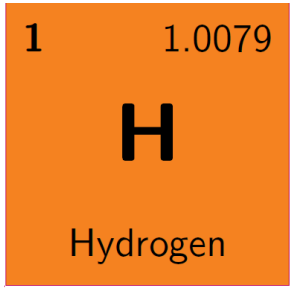
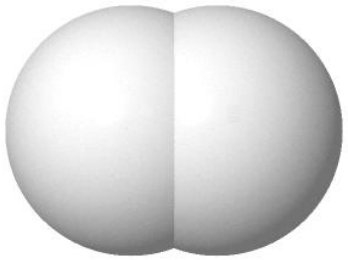
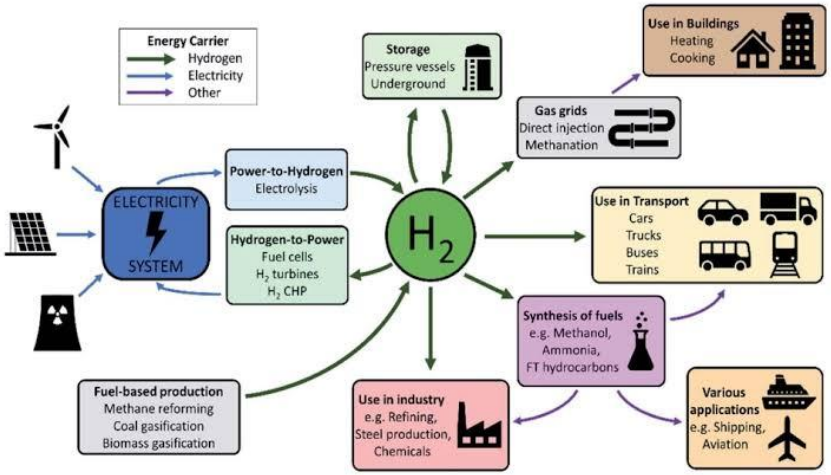




–H_2 is *an energy carrier* that is converted from primary energy sources into a secondary form, making it **storable** and **transportable**.



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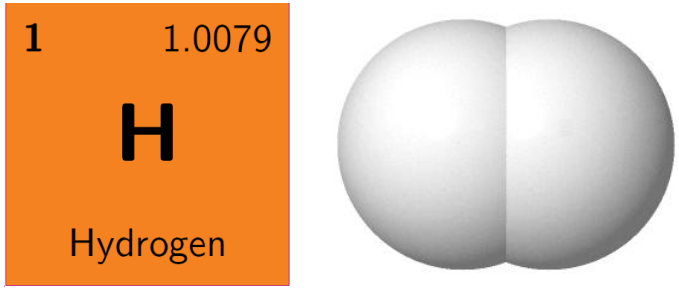
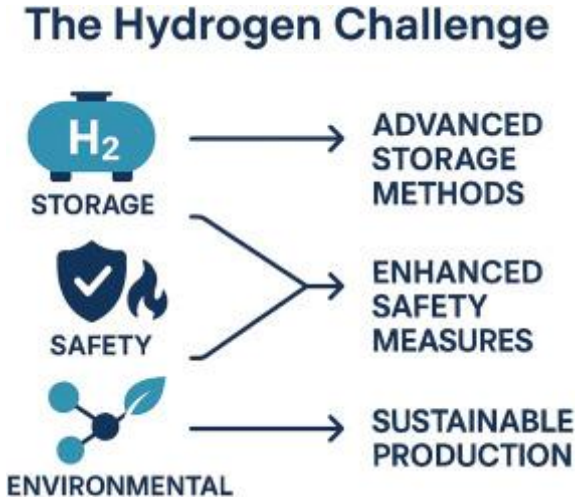
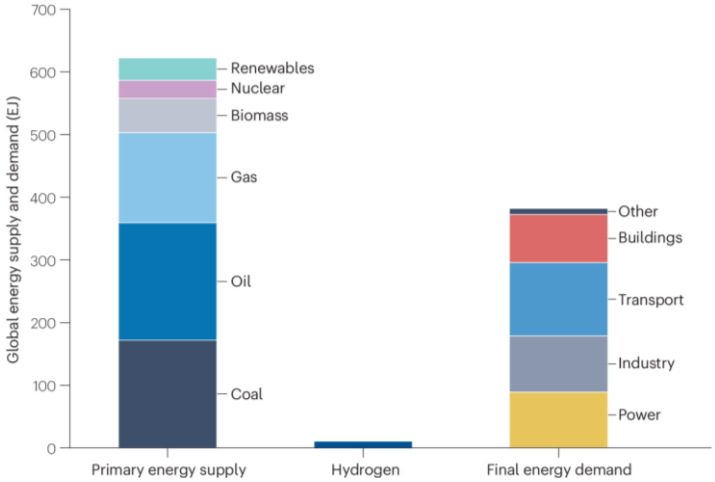
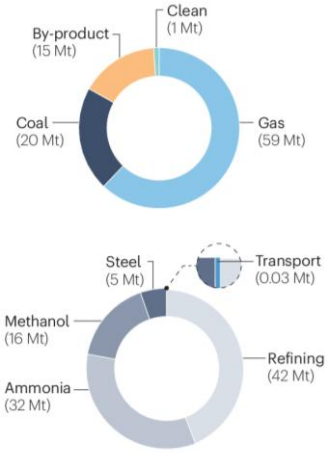


–Major challenges include production costs, storage limitations, the development of highly efficient combustion engines, and safety; **the economic viability needs be improved**.



Int. J. Hydrogen Energy, **167** (2025) 150952



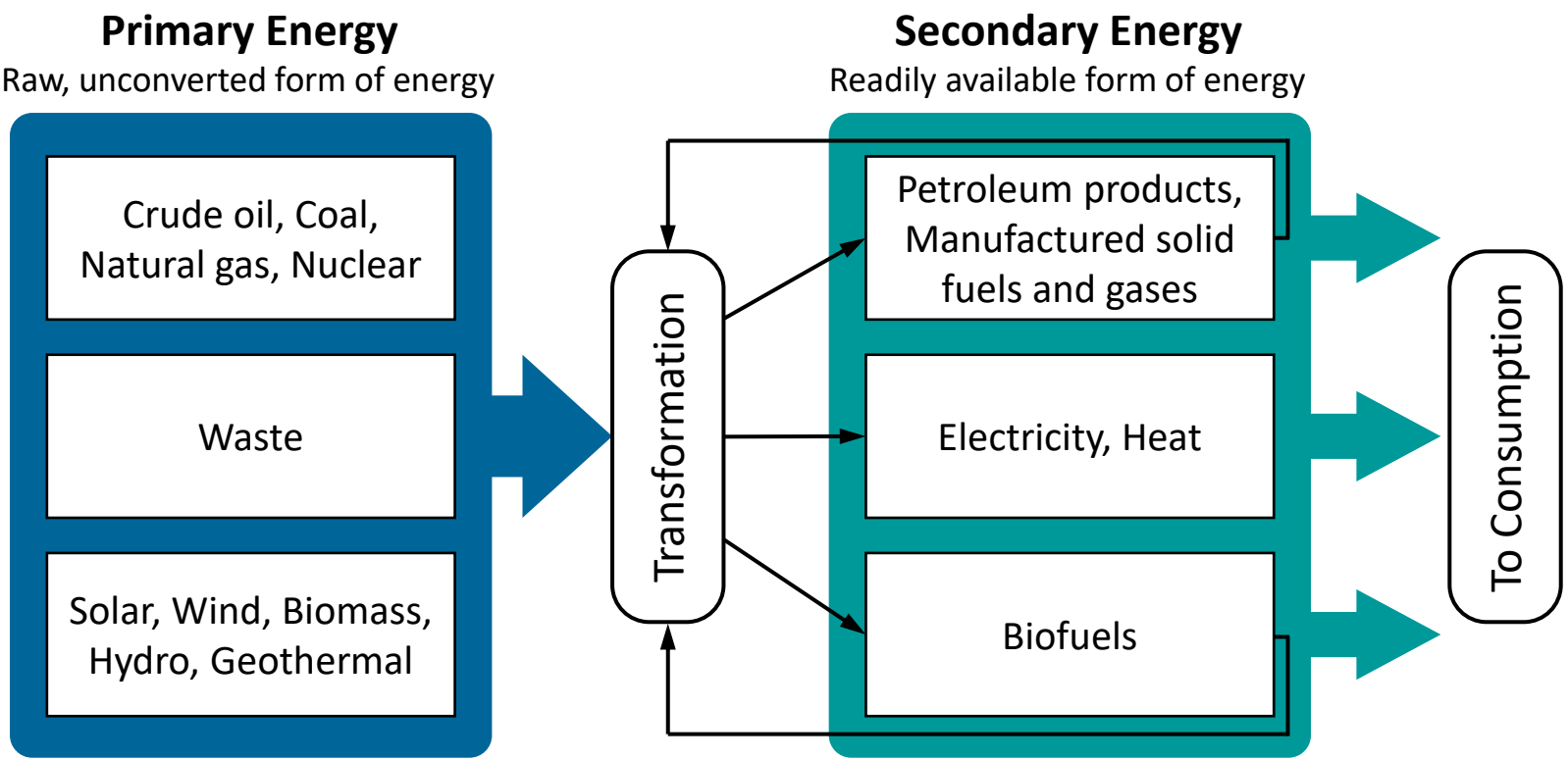


Nat. Rev. Clean Technol., **1** (2025) 351–371

Types of Energy

❑ Primary and Secondary Energy

Energy is indeed abundant, but *usable* energy is strictly limited, making *tools* essential



– *Usable* energy must be transformed from primary energy sources

– Every energy conversion process must entail *losses*

Renewable Energy

❑ Renewable Energy

Energy derived from natural resources that are replenished on a human timescale

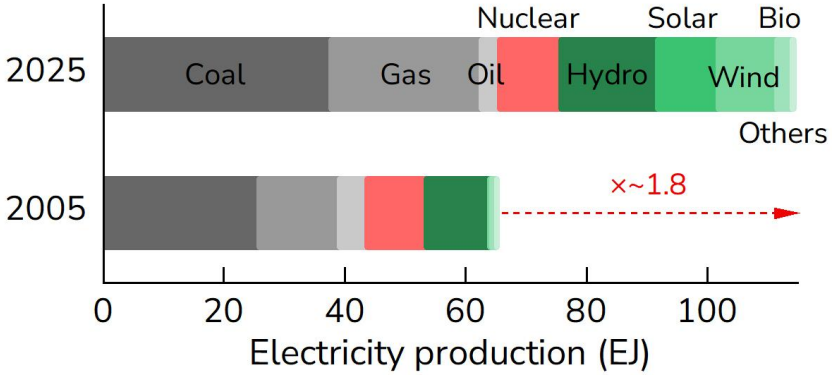
*Inexhaustible, Ubiquitous, Zero–CO_2 Emission

Solar Wind Hydropower Biomass Geothermal Heat

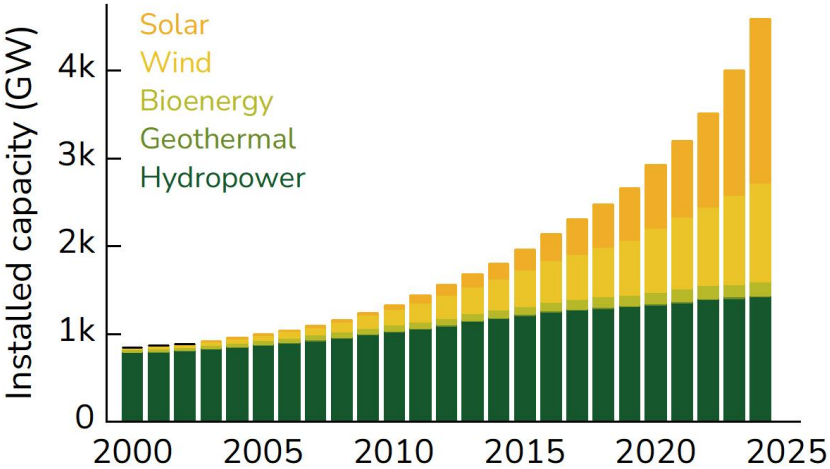
❑ Global Electricity Production

RE accounts for 34% in 2025 (18% in 2005)

*Others: geothermal, biomass, waste, wave and tidal



<Source: Statistical Review of World Energy (2025)>



<Source: IRENA (2025)>

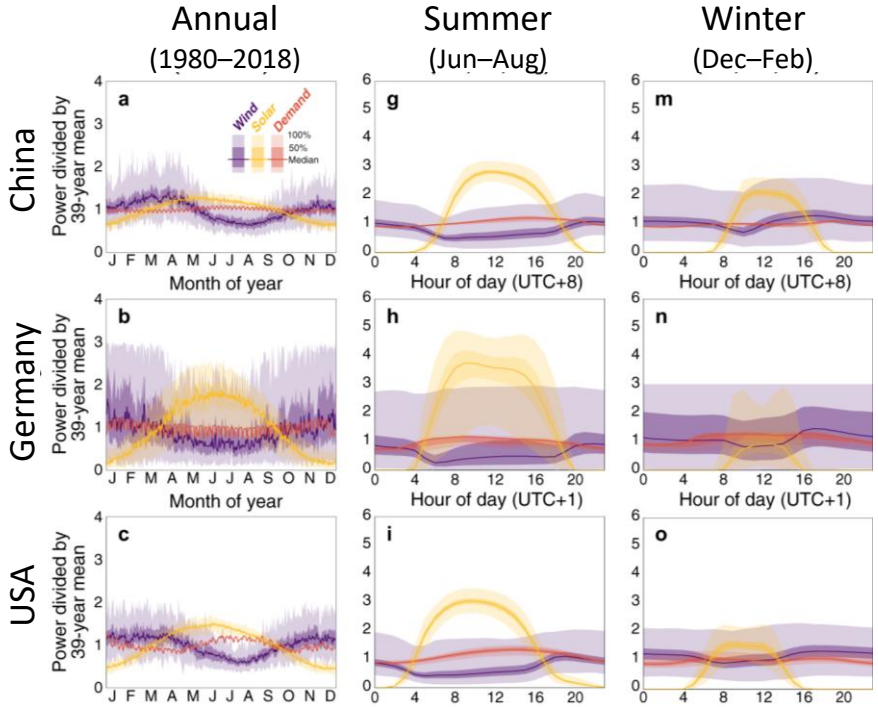
Challenges for Renewables

❑ Transport Issues

RE power generation sites are geographically distant from major urban consumption centers. Long–distance bulk power transmission suffers severe grid losses and infrastructure bottlenecks

❑ Storage Issues

RE power generation fluctuates based on weather and diurnal cycles. Electricity is difficult to store directly on a massive, long–term seasonal scale without loss.

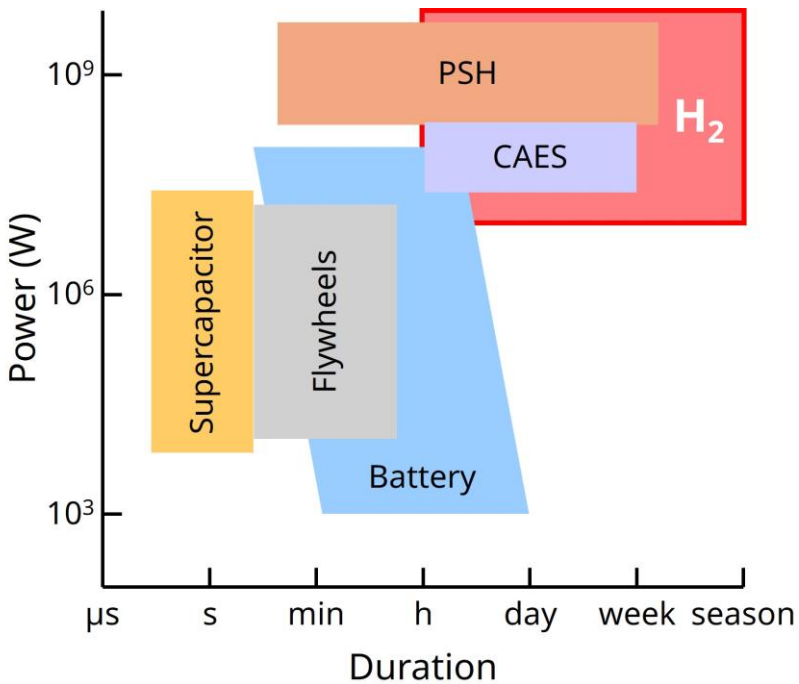


Nat. Comm., **12** (2021) 6146

Energy Storage System

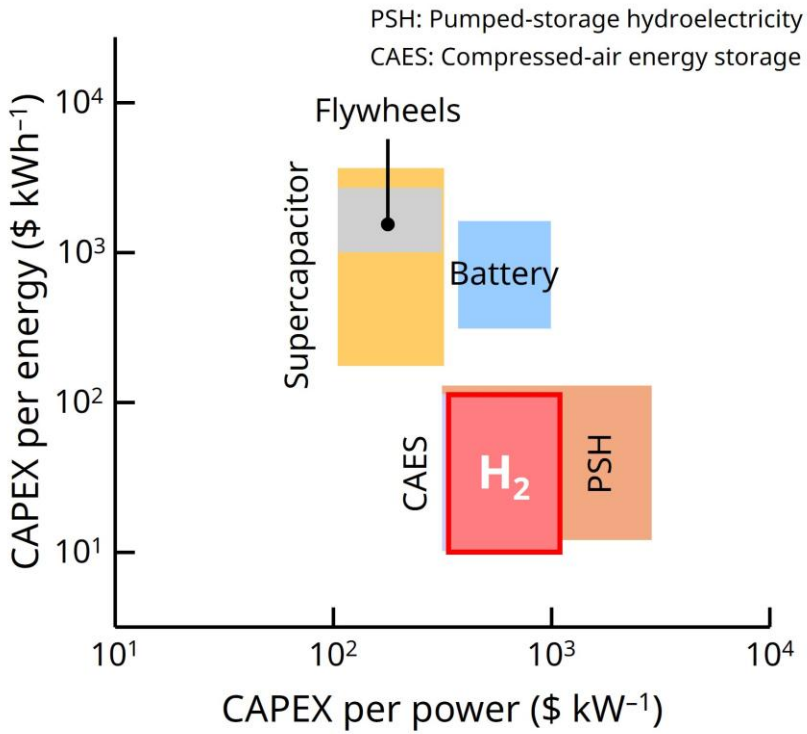
❑ Storage Capacity & Duration

- Long-duration storage
- High energy density in mass (120 MJ kg^{-1})



❑ Cost Effectiveness

- Low CAPEX per energy & power



<Source: IEA Technology Roadmap Hydrogen and Fuel Cells>

– H_2 has very high energy density in mass (120 (LHV) & 141.8 (HHV) MJ kg^{-1})

– H_2 can be transported in bulk and stored for long periods w/o degradation

Hydrogen Energy

❑ Renewable Energy

Energy derived from natural resources that are replenished on a human timescale

*Inexhaustible, Ubiquitous, Zero–CO_2 Emission

Solar | Wind | Hydropower | Biomass | Geothermal Heat

❑ Hydrogen Energy

Energy obtained as heat or power by combusting compounds that contain H or processing them through energy conversion systems

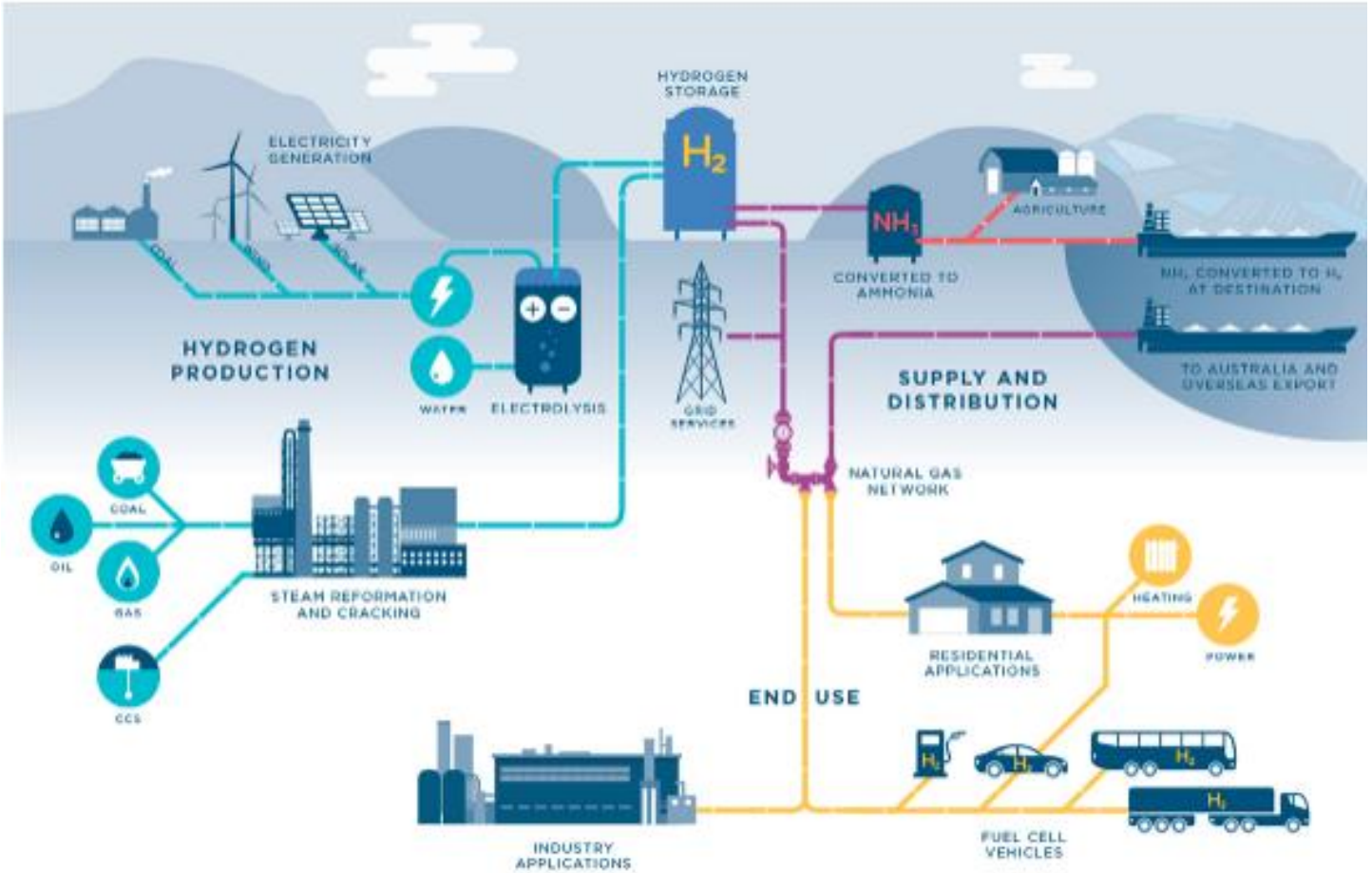
- Interoperability with Electricity
- Capability to Coupling with Renewable Energy

H_2 is highly interchangeable with electricity via fuel cells and electrolyzers. Thus, it enables full utilization and balancing of intermittent renewables.

Hydrogen Supply Chain

❑ Produce, store/transport, and use

Establishing, standardizing, and commercializing secure, low–cost technologies across these *three primary pillars* is essential for introducing a full hydrogen society



<Source: https://snurecl.com/>

Key Technological Objectives

❑ Produce, store/transport, and use

Establishing, standardizing, and commercializing secure, low–cost technologies across these *three primary pillars* is essential for introducing a full hydrogen society

PRODUCE

- Low cost
- Large scale
- Carbon-free production

STORE & TRANSPORT

- High density
- Loss free
- Safe contaminant

USE

- High efficiency
- Clean energy
- Safe energy

Key Technological Objectives

❑ Produce, store/transport, and use

Establishing, standardizing, and commercializing secure, low–cost technologies across these *three primary pillars* is essential for introducing a full hydrogen society

PRODUCE

- Low cost
- Large scale
- Carbon-free production

STORE & TRANSPORT

- High density
- Loss free
- Safe contaminant

USE

- Highly efficient device
- Clean energy

Global Hydrogen Production

❑ Grey, Blue, and Green Hydrogen

The world relies on fossil fuels (grey hydrogen), which account for ~98% of hydrogen production

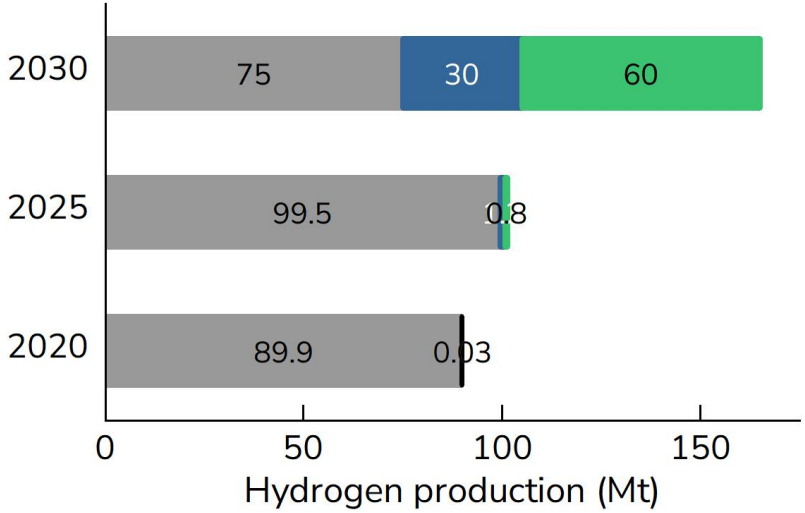
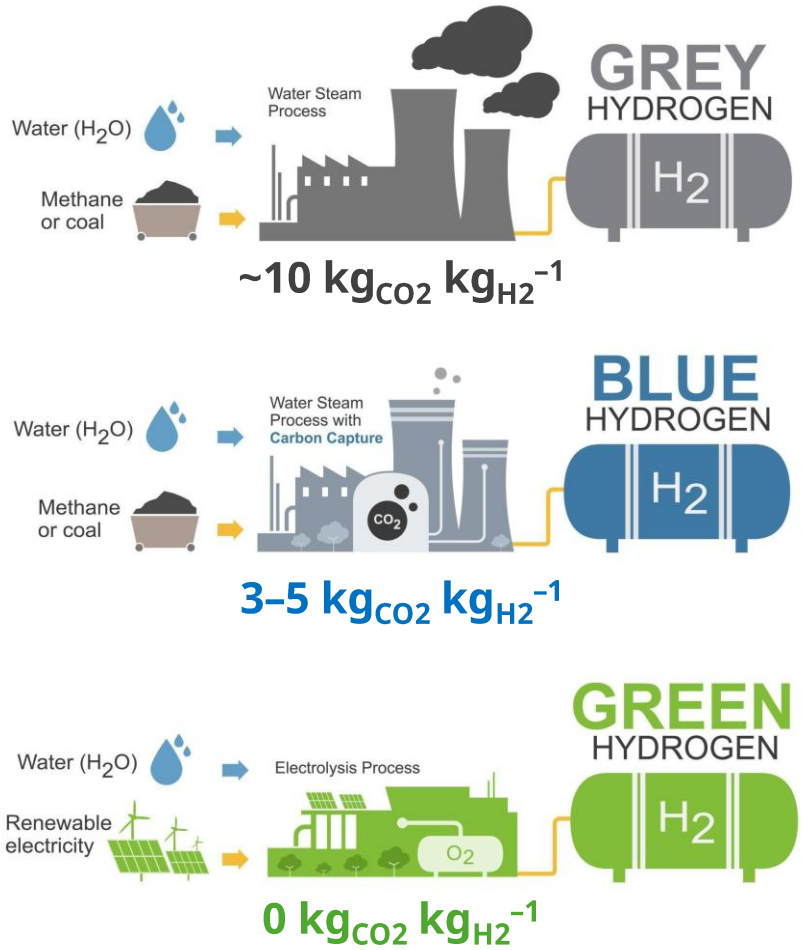


Table Levelized cost of hydrogen (USD kg^{-1})

	2020	**2025**	2030
Grey	1.0–2.5	**1.5–3.0**	1.5–3.2
Blue	1.5–3.0	**2.0–3.8**	1.8–3.5
Green	3.5–7.5	**4.5–8.5**	1.5–4.5

<Source: IEA (2025)>



Global Hydrogen Production

❑ Grey, Blue, and Green Hydrogen (2025)

The world relies on fossil fuels (grey hydrogen), which account for ~98% of hydrogen production

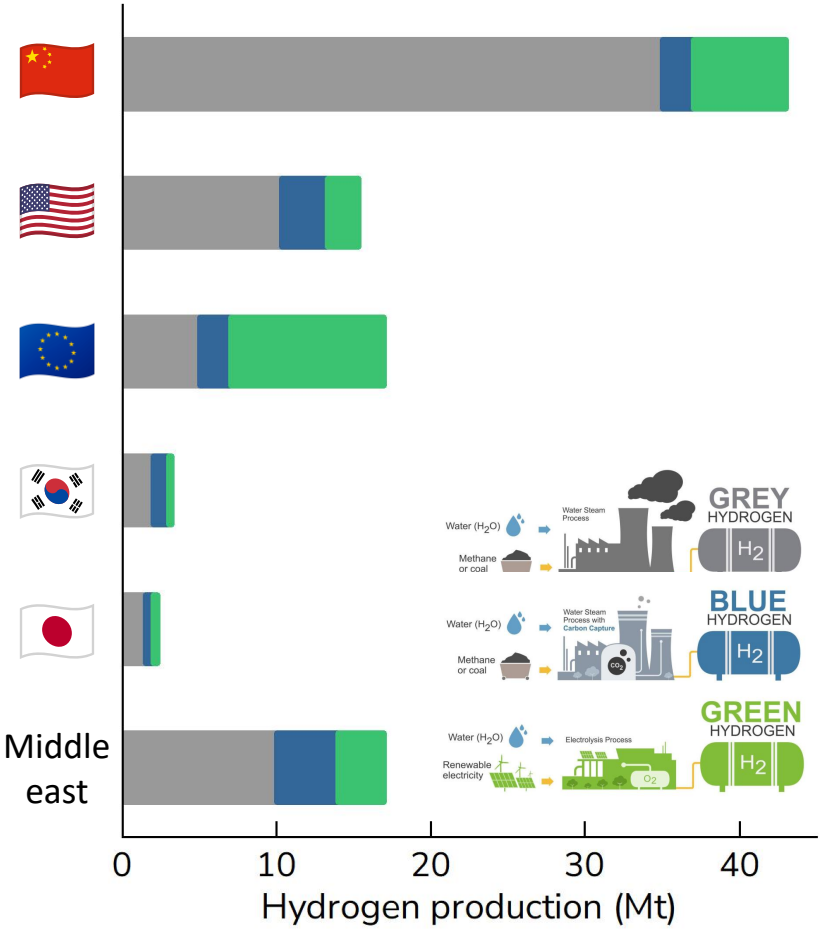
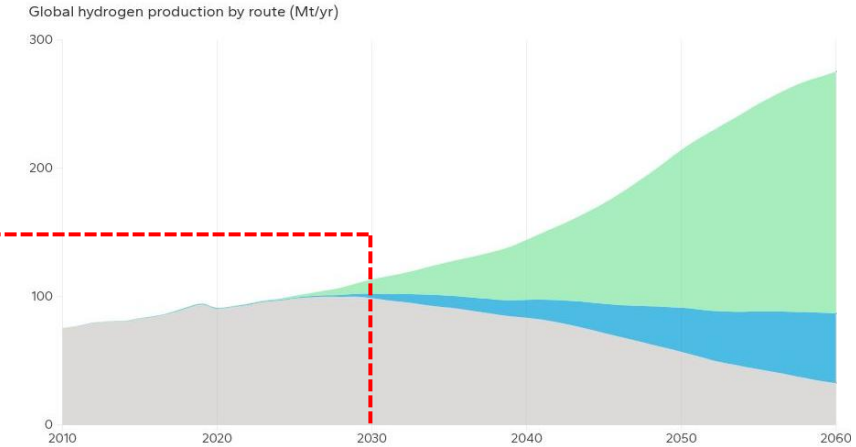
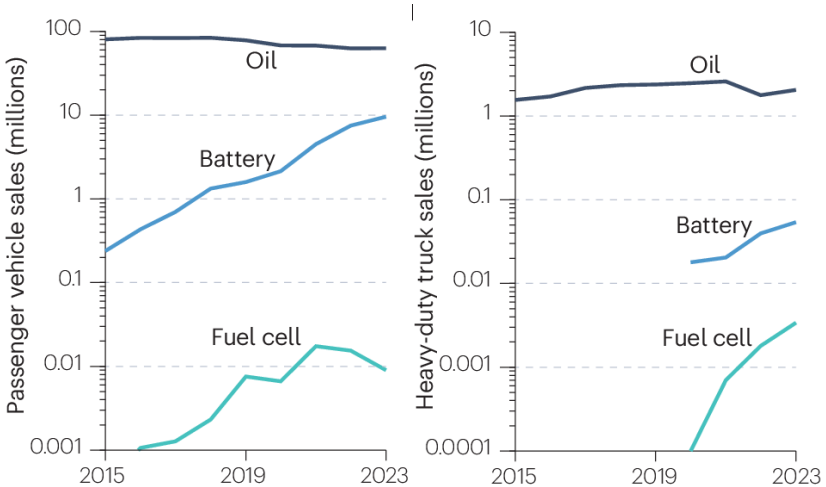


Fig. Hydrogen production prospects to 2030

<Source: IEA (2025)>



<Source: Energy Transition Outlook (2026)>



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Domestic Hydrogen Production

❑ Annual H_2 Production (2025)

Annual H_2 production in S. Korea reached ~2.2 Mt in 2025, >99% of which is grey hydrogen

기업		내용
HYUNDAI	현대차	수소전기차, 수소연료전지시스템 생산·판매
SK	SK	수소 밸류체인(생산·유통·소비) 구축, 수소충전소 운영
POSCO	포스코	수소 생산·판매
HYOSUNG	효성	수소 생산·유통, 수소충전소 운영
Hanwha	한화	수소 밸류체인 구축
DOOSAN	두산	수소연료전지 사업, 수소 생산·유통, 수소드론 판매
현대중공업	현대중공업	수소 밸류체인 구축
LOTTE	롯데	수소 생산·판매, 수소충전소 설치, 수소저장탱크 사업
GS	GS	수소 공급, 수소연료전지발전 구축
KOLON	코오롱	수소차 연료전지부품 생산·판매

- Byproduct (62.3%, ~1.4 Mt)
- Steam reforming (36.4%, ~0.80 Mt)
- Low- and/or zero-carbon (0.91%, ~0.020 Mt)

Domestic Hydrogen Production

❑ Byproduct Hydrogen

Oil Refinery in Ulsan

- 3rd largest in the world
- Ownership: SK Energy
- Capacity: 40.2 Mt yr^{-1} & 850,000 bpd
  *1 barrel = 159 L
- Products: LPG, Gasoline, Diesel, Jet fuel, Asphalt

Oil Refinery in Yeosu

- 5th largest in the world
- Ownership: GS Caltex (50% GS Holdings + 50% Chevron)
- Capacity: 730,000 bpd
- Products: Heavy Oil Upgrade (Gasoline, Kerosene, Naphtha)

– Large-scale refining & reforming processes generate abundant byproduct hydrogen

Domestic Hydrogen Production

❑ Steam Methane Reforming (SMR)

SMR Plant in Pyeongtaek

- Largest scale in Korea
- Ownership: KOGAS, HyNet, etc.
- Capacity: 2,550 t yr^{-1} (7 t day^{-1})
- Products: High-purity compressed H_2 for mobility, Tube trailers

SMR Plant in Changwon

- 1st commercial liquefied hydrogen plant
- Ownership: Doosan Enerbility, etc.
- Capacity: 1,800 t yr^{-1} (5 t day^{-1})
- Products: Liquefied Hydrogen, High-purity gas for buses, power generation

– NG-based SMR plants supply dedicated reformed H_2 for urban and regional mobility

Domestic Hydrogen Production

❑ Water Electrolysis

Water Electrolysis Plant in Jeju

- Largest facility in Korea (12.5 MW)
- Ownership: Korea Southern Power, etc.
- Capacity: 1,176 t yr^{-1} (up to ~250 kg h^{-1})
- Products: High-purity H_2 for FCVs, buses, and tube trailers

Water Electrolysis Plant in Buan

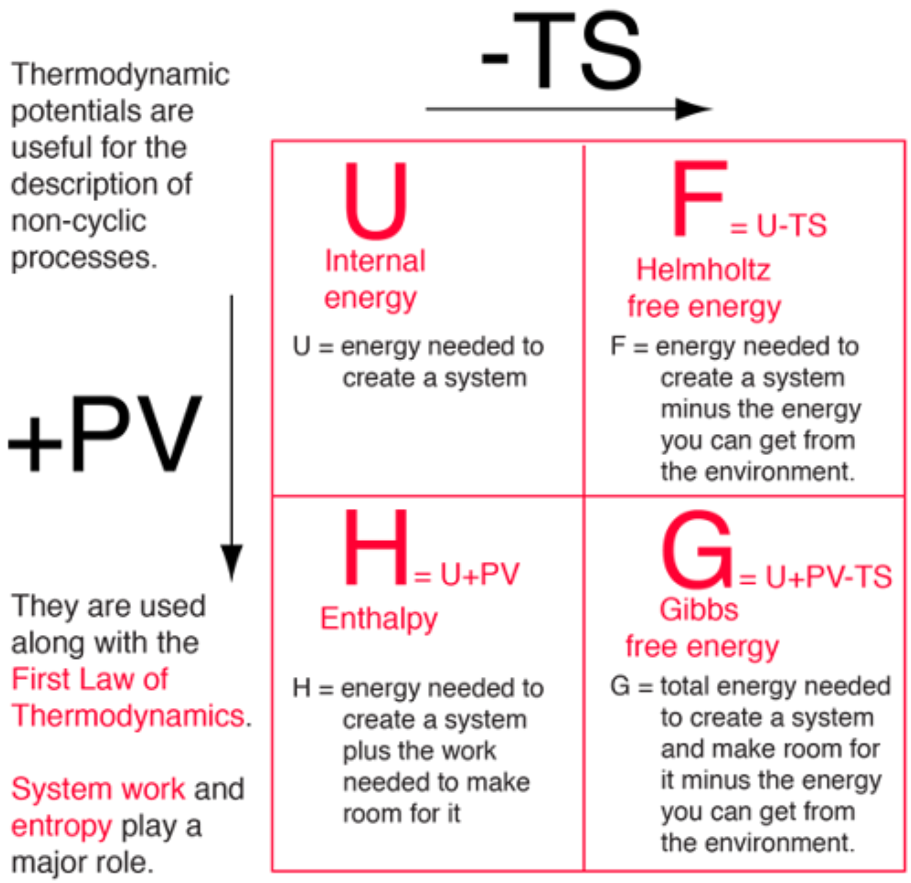
- Commercial MW-scale water electrolysis demonstration plant (2.5 MW)
- Ownership: Hyundai E&C, etc.
- Capacity: 365 t yr^{-1} (1 t day^{-1})
- Products: Green H_2 for local mobility, regional storage & distribution

– Renewable-based water electrolysis plants supply zero-carbon green H_2 for public transport and carbon neutrality demonstration

Basic of Thermodynamics

❑ Thermodynamic Potential

A scalar quantity used to represent the thermodynamic state of a system and measure the maximum reversible work or energy available from it under specific constraint conditions



Basic of Thermodynamics

❑ Enthalpy H (= $H(S, p) = U + pV$)

The sum of a thermodynamic system's internal energy and the product of its pressure and volume

- **Enthalpy Change ΔH**

  According to the 1st and 2nd laws of thermodynamics,

  $dU = \delta Q - \delta W$

  $\delta Q = TdS$

  (δQ: energy added as heat

  T: temperature

  dS: infinitesimal change)

  If only pV work is done, $\delta W = pdV$

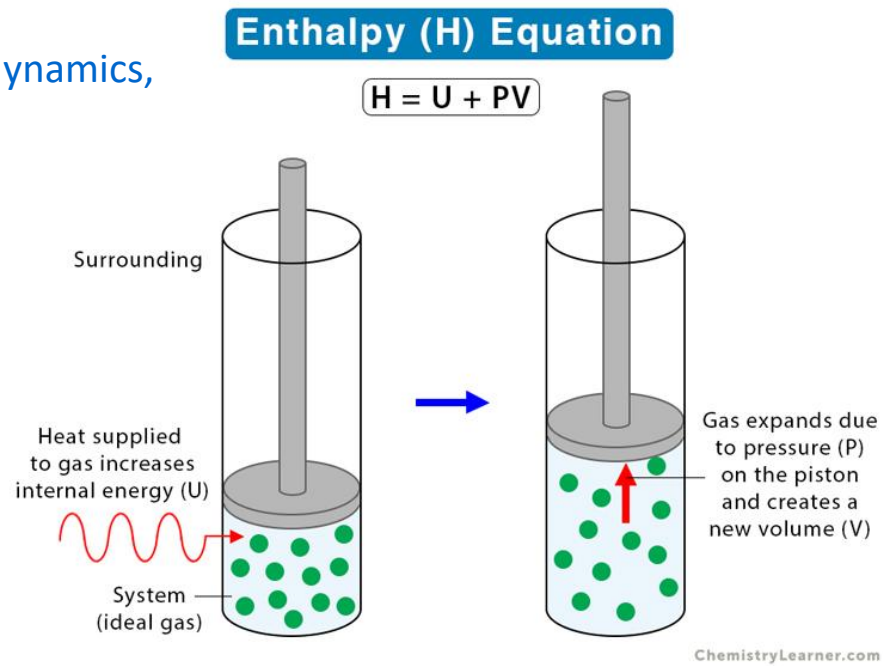
  $dU = TdS - pdV$

  $= TdS - pdV - Vdp + Vdp$

  $\Leftrightarrow dU + d(pV) = TdS + Vdp$

  $\therefore$ $\mathbf{dH = TdS + Vdp}$

  When $dp = 0$ (isobaric) then $dH = TdS = \delta Q$



ΔH is used to predict the heat of reaction, as reactions at atmospheric pressure are isobaric processes

Basic of Thermodynamics

❑ Enthalpy *H*

The sum of a thermodynamic system's internal energy and the product of its pressure and volume

- **Standard Reaction Enthalpy ΔH^o_{rxn}**
  The difference between total product and total reactant molar enthalpies, calculated for substances in their standard states (25°C, 1 atm).

  For a generic chemical reaction
  $v_A A + v_B B + \ldots \rightarrow v_X X + v_Y Y + \ldots,$

  ΔH^o_{rxn} is related to the standard enthalpy of formation $\Delta_f H^o$ of the reactants and products;
  $$\Delta H^o_{rxn} = \Sigma v_{product} \Delta_f H^o_{product} - \Sigma v_{reactant} \Delta_f H^o_{reactant}$$
  , where v_i is the stoichiometric coefficients of each product and reactant.

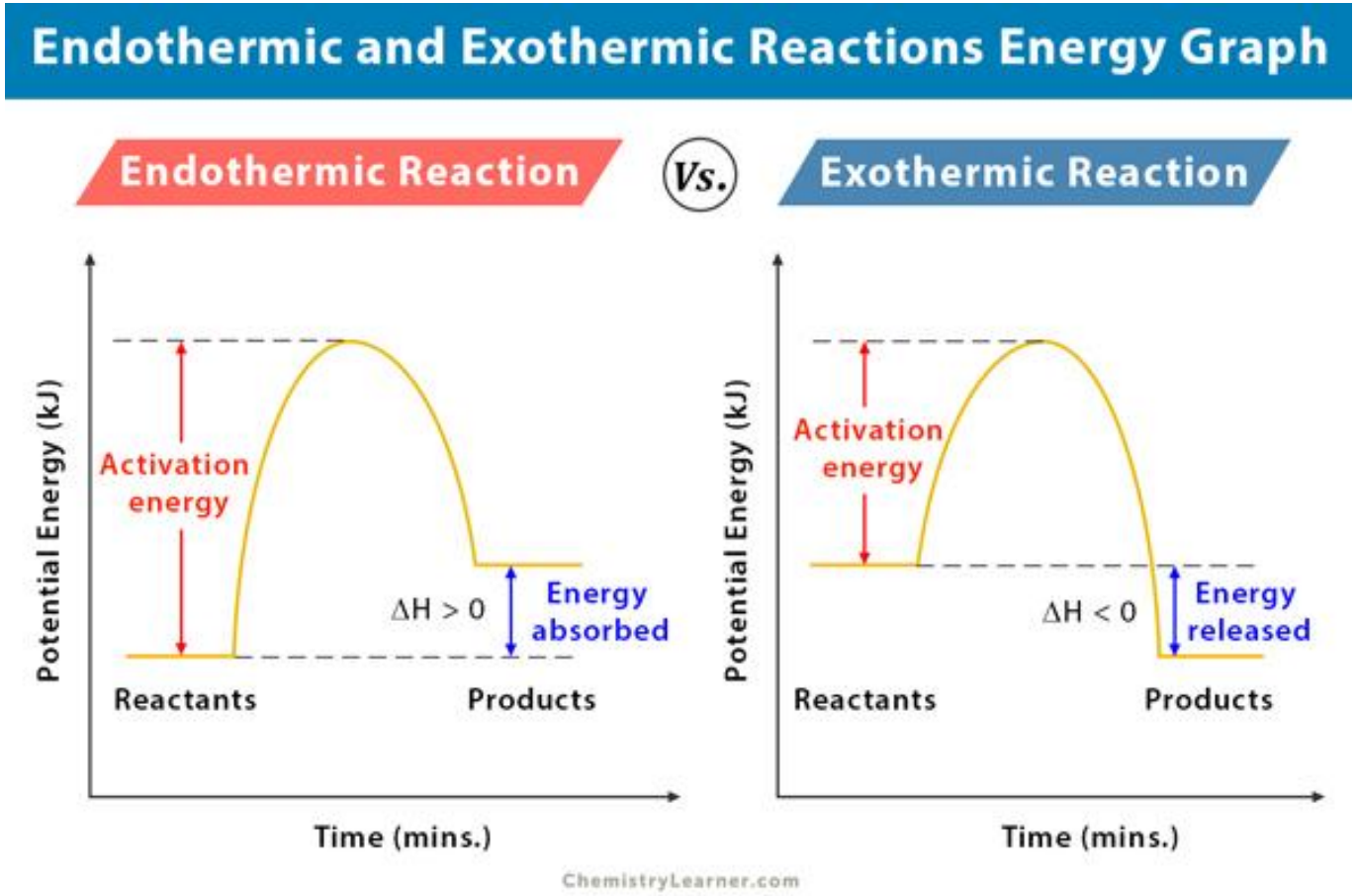
Basic of Thermodynamics

❑ Exothermic and Endothermic Reactions

When $\Delta H < 0$: Exothermic reaction (e.g., Combustion)

$\Delta H = 0$: No net change in enthalpy

$\Delta H > 0$: Endothermic reaction (e.g., Ice melting)



Basic of Thermodynamics

❑ Helmholtz Free Energy F (= $F(T, V) = U - TS$)

The useful work obtainable from a closed thermodynamic system at a constant temperature

- **Helmholtz Free Energy Change ΔF**

  According to the 1st and 2nd laws of thermodynamic

  $dU = \delta Q - \delta W$

  $\delta Q = TdS$

  (δQ: energy added as heat

  T: temperature

  dS: infinitesimal change)

  If only pV work is done, $\delta W = pdV$

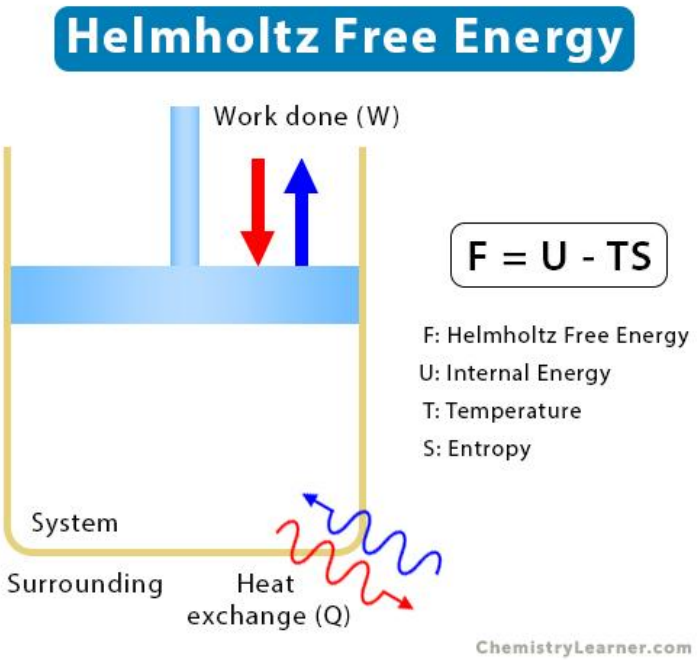
  $dU = TdS - pdV$

  $= TdS - pdV + SdT - SdT$

  $\Leftrightarrow dU - d(TS) = -SdT - pdV$

  $\therefore$ $\mathbf{dF = -SdT - pdV}$

  When $dT = 0$ (isothermal) then $dF = -pdV = -\delta W$



Basic of Thermodynamics

❑ Gibbs Free Energy G (= $G(p, T) = U + pV - TS = H - TS$)

The maximum amount of work that may be performed by a thermodynamically closed system at constant temperature and pressure

- **Gibbs Free Energy Change ΔG**

  According to the 1st law of thermodynamics,

  $dU = \delta Q - \delta W$

  The work done on the system can be written by

  $\delta W = pdV + \delta W_x$

  (δW_x: other forms of work (electrical, magnetic, etc.))

  Then

  $dU = \delta Q - pdV - \delta W_x$

  And

  $\mathbf{dG} = dU + pdV - TdS$

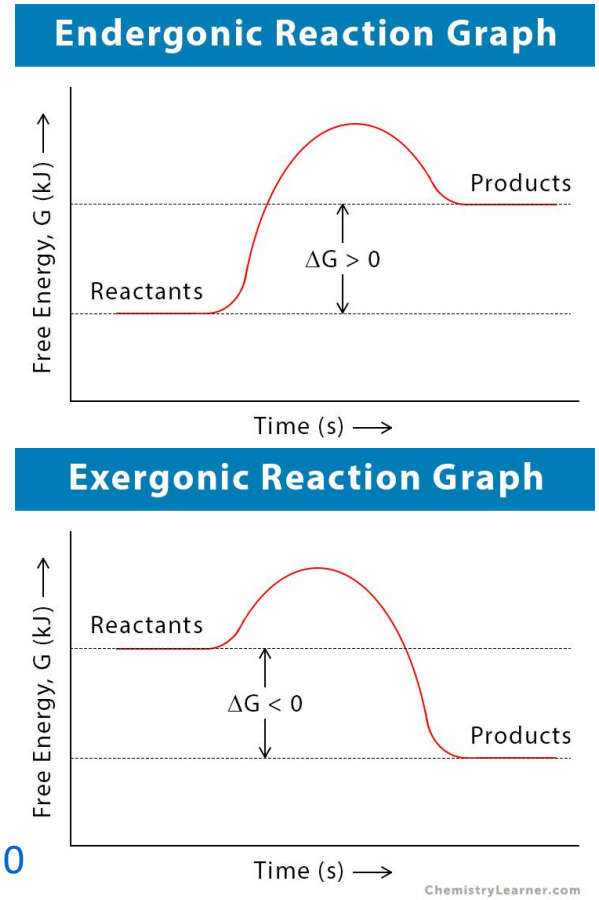
  $= \mathbf{dH - TdS}$

  $= \delta Q - TdS - \delta W_x$

According to the 2nd law of thermodynamics ($\delta Q \leq TdS$),

$dG \leq \delta W_x$

When $\delta W_x = 0$ (if only mechanical work is done) then $dG \leq 0$



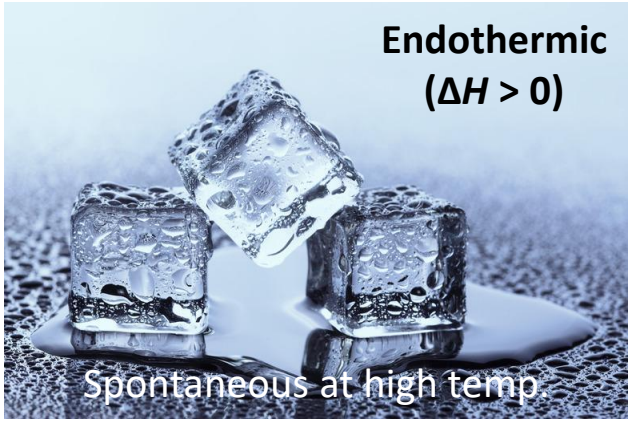
Basic of Thermodynamics

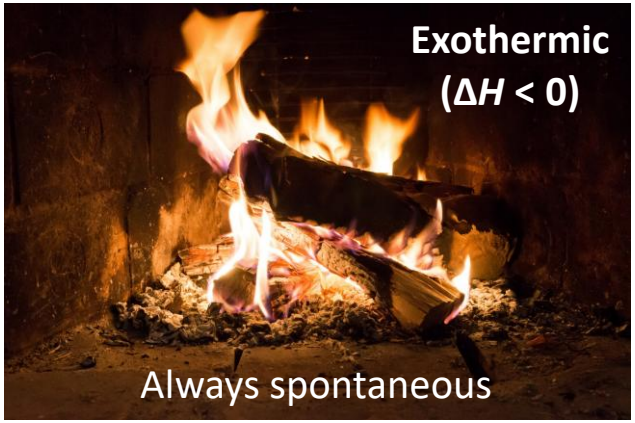
❑ Exergonic and Endergonic Reactions

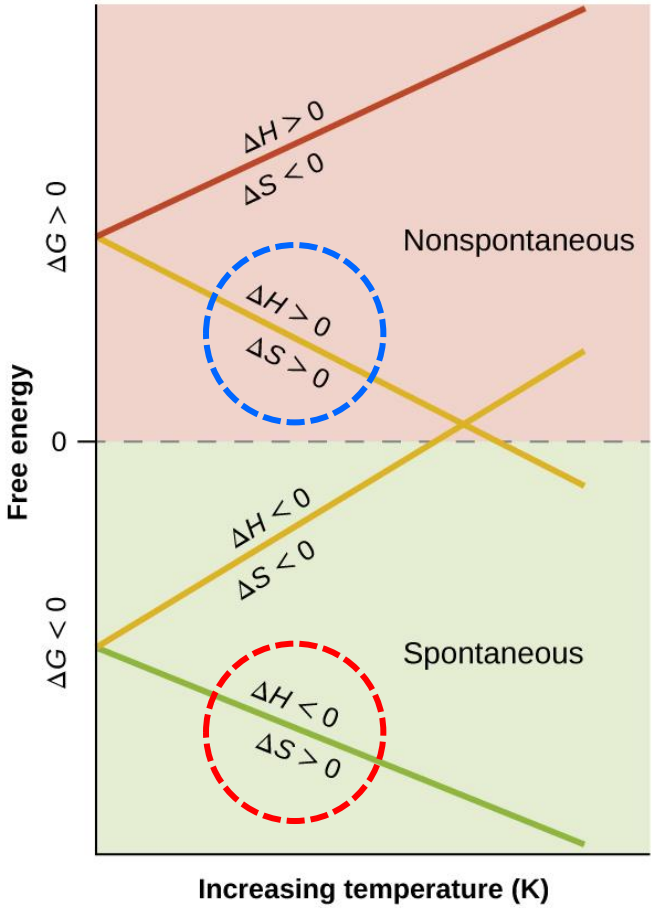
When $\Delta G < 0$: The forward reaction happens by itself; it releases energy (exergonic)

$\Delta G = 0$: Equilibrium

$\Delta G > 0$: The forward reaction does not happen by itself; it needs an energy input (endergonic)







Hydrogen Energy

❑ Oxidation of Methanol

The reaction of burning methanol with oxygen to produce carbon dioxide and liquid water

- Direct methanol fuel cells (DMFCs) use methanol instead of hydrogen as fuel.
  Calculate the standard enthalpy ΔH^o and standard entropy ΔS^o for the methanol combustion reaction at 25 °C, 1 atm.

$$CH_3OH(l) + 1.5O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$$

Chemical species	$\Delta_f H^o$ (kJ mol^{-1})	$\Delta_f S^o$ (J mol^{-1} K^{-1})
$CH_3OH(l)$	–238.5	127.2
$O_2(g)$	0	205.0
$CO_2(g)$	–393.5	213.8
$H_2O(l)$	–285.8	69.95

$$\Delta H^o_{rxn} = \Sigma v_{product}\Delta_f H^o_{product} - \Sigma v_{reactant}\Delta_f H^o_{reactant}$$

kJ mol^{-1}

= kJ mol^{-1}

$$\Delta S^o_{rxn} = \Sigma v_{product}\Delta_f S^o_{product} - \Sigma v_{reactant}\Delta_f S^o_{reactant}$$

=

J mol^{-1} K^{-1}

= J mol^{-1} K^{-1}

Hydrogen Energy

❑ Water–gas shift reaction

The reaction of carbon monoxide and water vapor to form carbon dioxide and hydrogen

- Determine the temperature at which the following reaction attains equilibrium.

$CO(g) + H_2O(g) \leftrightarrow CO_2(g) + H_2(g)$

Chemical species	$\Delta_f H^o$ (kJ mol^{-1})	$\Delta_f S^o$ (J mol^{-1} K^{-1})
$CO(g)$	–110.5	197.7
$H_2O(g)$	–241.8	188.8
$CO_2(g)$	–393.5	213.8
$H_2(g)$	0	130.7

$\Delta H^o_{rxn} = \Sigma v_{product} \Delta_f H^o_{product} - \Sigma v_{reactant} \Delta_f H^o_{reactant}$

= kJ mol^{-1}

= kJ mol^{-1}

$\Delta S^o_{rxn} = \Sigma v_{product} \Delta_f S^o_{product} - \Sigma v_{reactant} \Delta_f S^o_{reactant}$

= J mol^{-1} K^{-1}

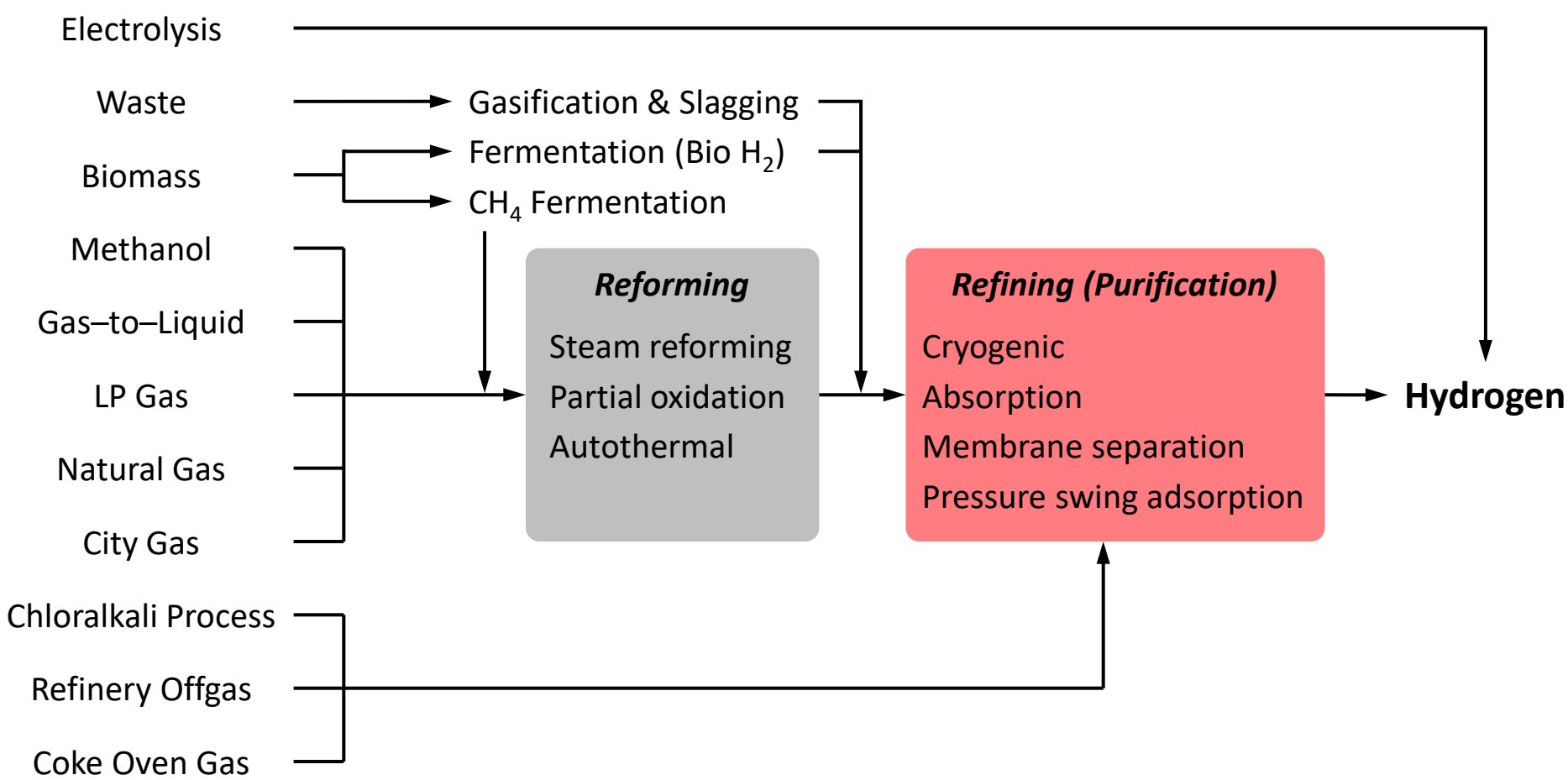
= J mol^{-1} K^{-1}

$\Delta G^o_{rxn} = \Delta H^o_{rxn} - T\Delta S^o_{rxn} = 0$

$\therefore T = \Delta H^o_{rxn} / \Delta S^o_{rxn} =$

Hydrogen Production

❑ Various Production Methods

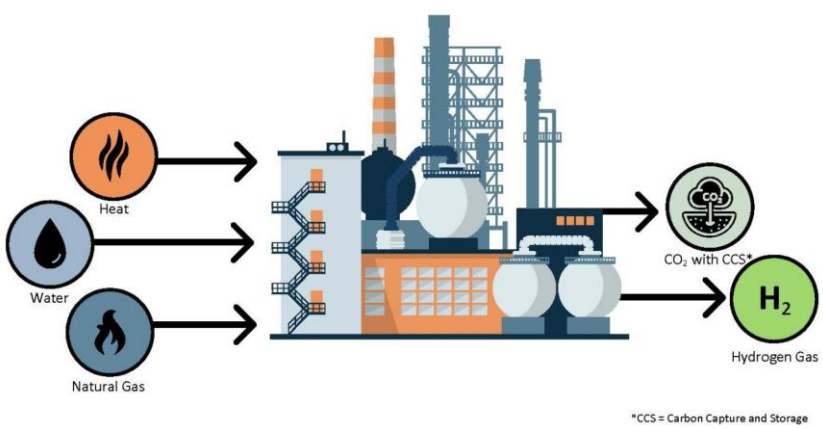


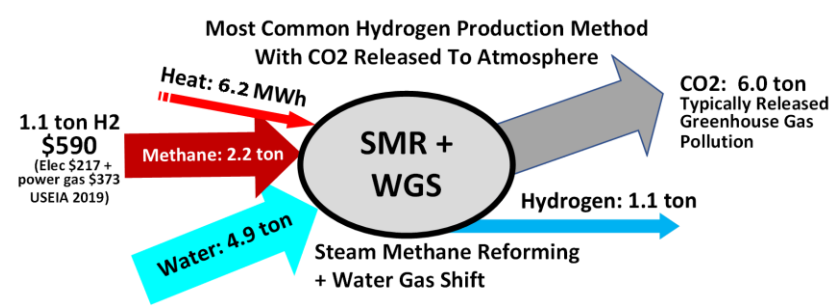
Reformed Hydrogen

❑ Steam Methane Reforming (SMR)

A method for producing syngas (H_2+CO) by reaction of hydrocarbon (e.g., NG) and water

- SMR is dominant method and accounts for ~60–75% of global hydrogen production
- $CH_4 + H_2O \rightarrow CO + 3H_2$ ($\Delta H° = 206.1$ kJ mol^{-1})
- CH_4 reacts with H_2O at high temperatures (700–1000 °C) & high pressures (3–25 bar)
- Then, water–gas shift reaction occurs (WGS) ($CO + H_2O \rightarrow CO_2 + H_2$ ($\Delta H° = -41.2$ kJ mol^{-1}))
- **Direct steam reforming** $CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$ ($\Delta H° = 164.9$ kJ mol^{-1})





<Source: https://www.energy.gov/media/292851>

<Source: https://en.wikipedia.org/wiki/Steam_reforming>

Reformed Hydrogen

❑ Steam Reforming of Hydrocarbon

- Write the balanced chemical equations for the direct steam reforming of propane (C_3H_8) and ethanol (C_2H_5OH). For each reaction, state the standard enthalpy of reaction ΔH^o and calculate the mass of CO_2 emitted to produce 1.0 kg of H_2.
  (Assume the molar masses of H_2 and CO_2 are respectively 2.0 and 44 g mol^{-1} for your calculations and round your final answers to one decimal places.)

Propane $C_3H_8 + H_2O \rightarrow CO + H_2$ (ΔH^o = 498.6 kJ mol^{-1}) (Steam reforming of C_3H_8)

$CO + H_2O \rightarrow CO_2 + H_2$ (ΔH^o = –41.2 kJ mol^{-1}) (Water–gas shift reaction)

$C_3H_8 + H_2O \rightarrow CO_2 + H_2$ (ΔH^o = kJ mol^{-1}) (Direct steam reforming of C_3H_8)

n_{CO2} = (1000 g ÷ 2.0 g mol^{-1}) ÷ = mol

∴ m_{CO2} = mol × 44 g mol^{-1} = kg

Reformed Hydrogen

❑ Steam Reforming of Hydrocarbon

- Write the balanced chemical equations for the direct steam reforming of propane (C_3H_8) and ethanol (C_2H_5OH). For each reaction, state the standard enthalpy of reaction ΔH^o and calculate the mass of CO_2 emitted to produce 1.0 kg of H_2.
  (Assume the molar masses of H_2 and CO_2 are respectively 2.0 and 44 g mol^{-1} for your calculations and round your final answers to one decimal places.)

Ethanol $C_2H_5OH + H_2O \rightarrow CO + H_2$ (ΔH^o = 256.1 kJ mol^{-1}) (Steam reforming of C_2H_5OH)

$CO + H_2O \rightarrow CO_2 + H_2$ (ΔH^o = –41.2 kJ mol^{-1}) (Water–gas shift reaction)

$C_2H_5OH + H_2O \rightarrow CO_2 + H_2$ (ΔH^o = kJ mol^{-1}) (Direct steam reforming of C_2H_5OH)

n_{H2} = (1000 g ÷ 2.0 g mol^{-1}) ÷ = mol

∴ m_{CO2} = mol × 44 g mol^{-1} = kg

Reformed Hydrogen

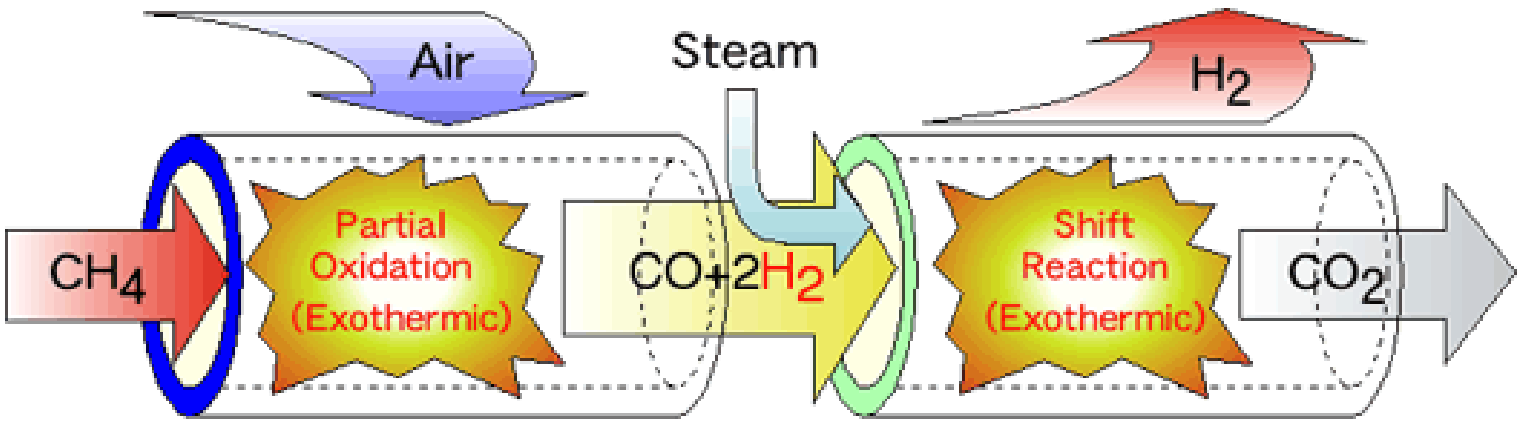
❑ Partial Oxidation (POX)

POX occurs when a substoichiometric fuel–air mixture is partially combusted in a reformer

- $C_nH_m + 0.5nO_2 \rightarrow nCO + 0.5mH_2$ ($\Delta H°_{POX} < 0$)

  (e.g., partial oxidation of methane: $CH_4 + 0.5O_2 \rightarrow CO + 2H_2$ ($\Delta H°_{POX} = -35.7$ kJ mol^{-1}))

  (cf., complete oxidation of methane: $CH_4 + 2O_2 \rightarrow CO_2 + H_2O$ ($\Delta H°_{COX} = -891$ kJ mol^{-1}))
- Subsequently, water–gas shift reaction occurs ($CO + H_2O \rightarrow CO_2 + H_2$ ($\Delta H°_{WGS} = -41.2$ kJ mol^{-1}))
- POX is much faster than SMR and requires a smaller reactor vessel



<Source: https://ceram.material.tohoku.ac.jp/~takamura/research_opm_e.html>

Reformed Hydrogen

❑ Partial Oxidation (POX)

- Write the overall balanced chemical equations combining POX and WGSR for propane (C_3H_8) and ethanol (C_2H_5OH). For each overall process, state the standard enthalpy of reaction ΔH^o and calculate the mass of CO_2 emitted to produce 1.0 kg of H_2.
  (Assume the molar masses of H_2 and CO_2 are respectively 2.0 and 44 g mol^{-1} for your calculations and round your final answers to one decimal places.)

Propane $C_3H_8 + \quad O_2 \rightarrow \quad CO + \quad H_2$ ($\Delta H^o = -226.8$ kJ mol^{-1}) (Partial oxidation of C_3H_8)

$CO + H_2O \rightarrow CO_2 + H_2$ ($\Delta H^o = -41.2$ kJ mol^{-1}) (Water–gas shift reaction)

$C_3H_8 + \quad O_2 + \quad H_2O \rightarrow \quad CO_2 + \quad H_2$ ($\Delta H^o =$ kJ mol^{-1}) (Overall)

n_{CO2} = (1000 g ÷ 2.0 g mol^{-1}) ÷ = mol

∴ m_{CO2} = mol × 44 g mol^{-1} = kg

Reformed Hydrogen

❑ Partial Oxidation (POX)

- Write the overall balanced chemical equations combining POX and WGSR for propane (C_3H_8) and ethanol (C_2H_5OH). For each overall process, state the standard enthalpy of reaction ΔH^o and calculate the mass of CO_2 emitted to produce 1.0 kg of H_2.
  (Assume the molar masses of H_2 and CO_2 are respectively 2.0 and 44 g mol^{-1} for your calculations and round your final answers to one decimal places.)

Ethanol $C_2H_5OH + \quad O_2 \rightarrow \quad CO + \quad H_2$ (ΔH^o = 13.8 kJ mol^{-1}) (Partial oxidation of C_2H_5OH)

$CO + H_2O \rightarrow CO_2 + H_2$ (ΔH^o = –41.2 kJ mol^{-1}) (Water–gas shift reaction)

$C_2H_5OH + \quad O_2 + \quad H_2O \rightarrow \quad CO_2 + \quad H_2$ (ΔH^o = kJ mol^{-1}) (Overall)

n_{CO2} = (1000 g ÷ 2.0 g mol^{-1}) ÷ = mol

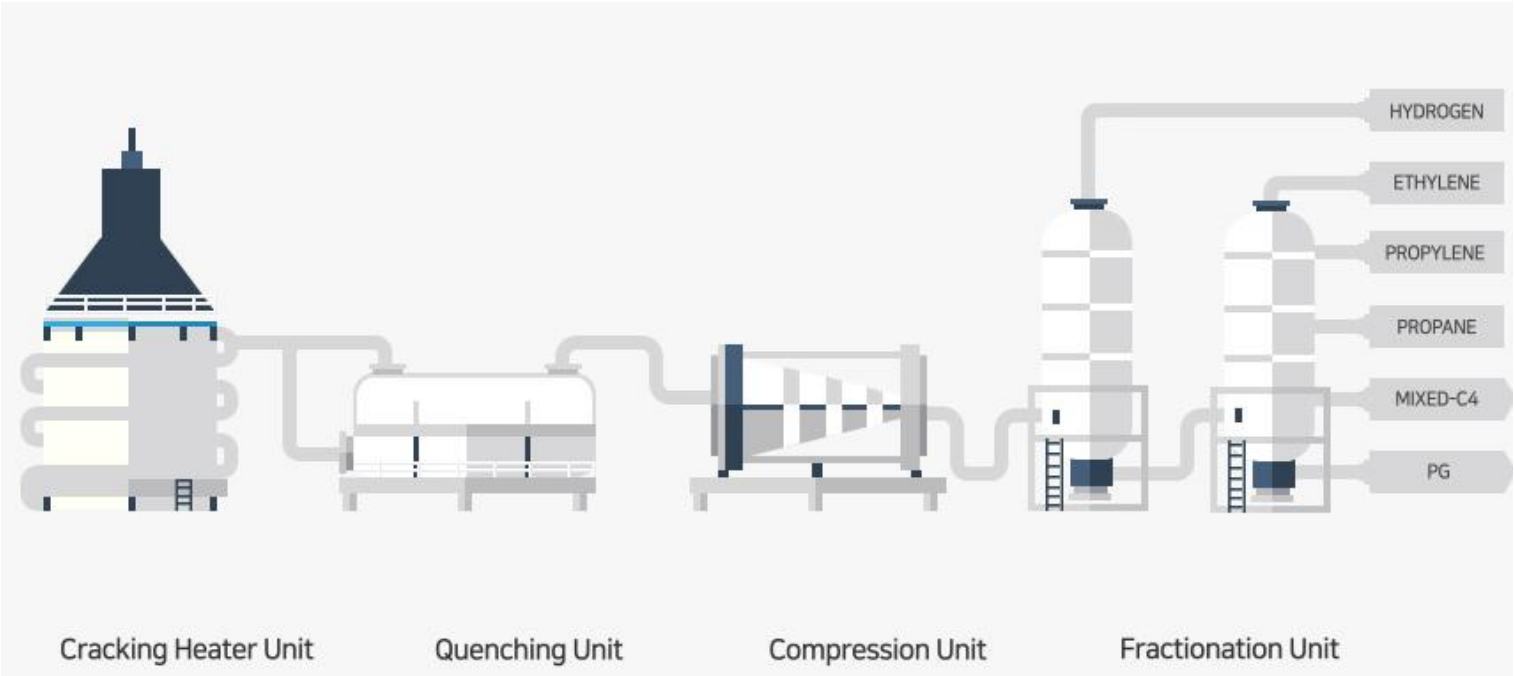
∴ m_{CO2} = mol × 44 g mol^{-1} = kg

Byproduct Hydrogen

❑ Hydrocarbon Steam Cracking

Pyrolysis of hydrocarbons (naphtha, ethane, LPG, gas oil, etc.) produces byproduct hydrogen along with basic petrochemicals (ethylene, propylene, propane, etc.), followed by purification using deep cryogenic distillation (boiling point differences).

- **Internal**: Fuel for cracking furnaces, selective hydrogenation of alkynes
  *$C_2H_2 + H_2 \rightarrow C_2H_4$ (Ethylene)
- **External**: Hydrodesulfurization in oil refineries, industrial fuel, or chemical reduction processes
  **$Fe_2O_3 + 3H_2 \rightarrow 2Fe + 3H_2O$



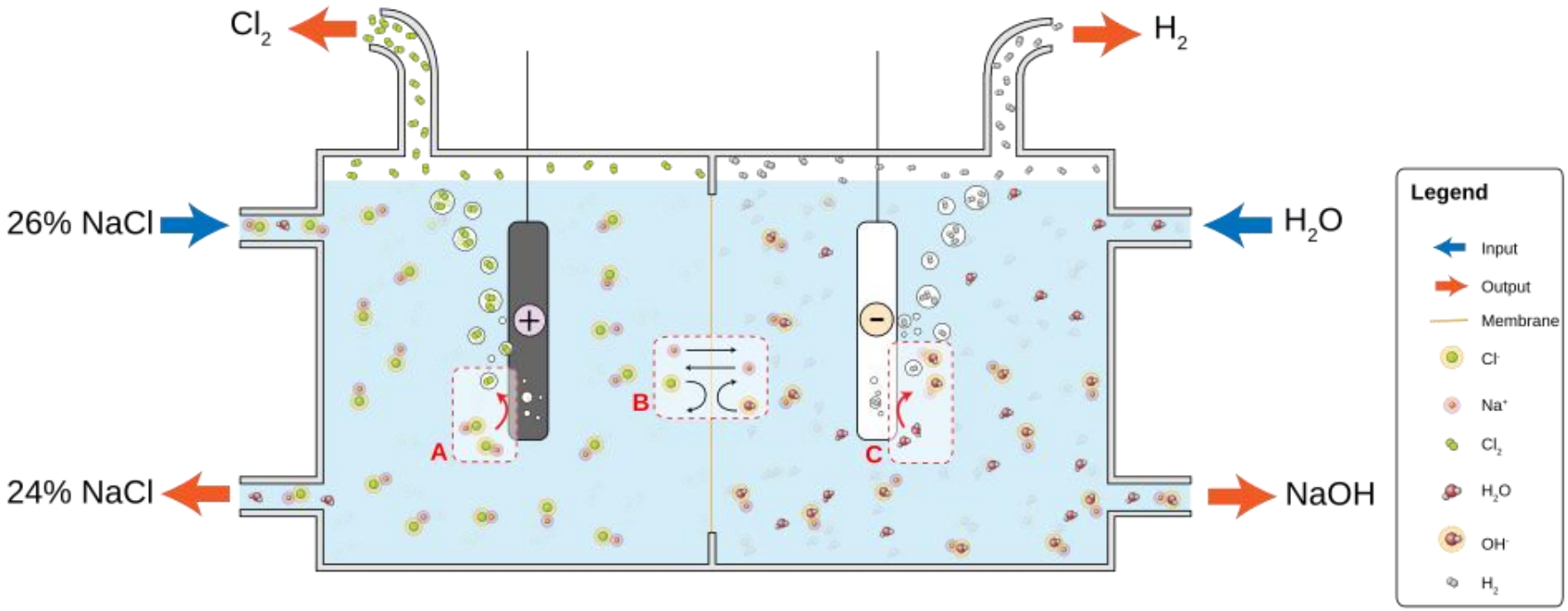
<Source: https://www.yncc.co.kr/en/product/factory/3/ethylene.do>

Byproduct Hydrogen

❑ Chloralkali Process

Electrolysis of sodium chloride (NaCl) solutions (e.g., brine (high-conc. solution of salt in water))

- $2NaCl + H_2O \rightarrow Cl_2 + H_2 + 2NaOH$
- 97 Mt of Cl_2 were prepared in 2022 (35 Mt in 1987)
- To produce 1 t of NaOH, 2500 kWh of electricity is used with ~25 kg of H_2 as a byproduct



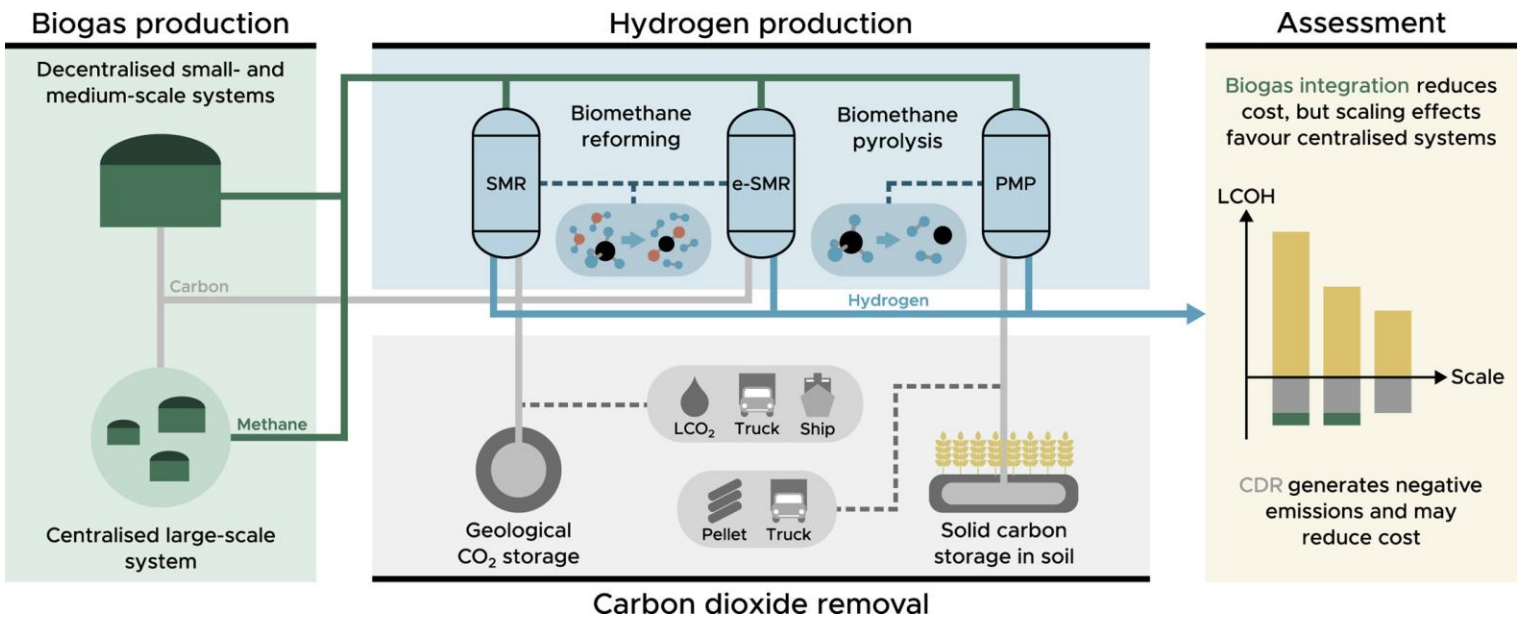
<Source: https://en.wikipedia.org/wiki/Chloralkali_process>

Biohydrogen

❑ Thermochemical Process (Biogas Reforming)

Obtained by reforming biogas, which is a mixture produced by microorganisms decomposing organic waste under anaerobic conditions (oxygen-free conditions)

- Upgrades raw biogas to high-purity CH_4 first by removing CO_2 and impurities, followed by SMR
- Emits CO_2 during the reforming step, requiring CCUS integration for zero-carbon certification
- e.g., Hyundai Motor, Hanwha E&C



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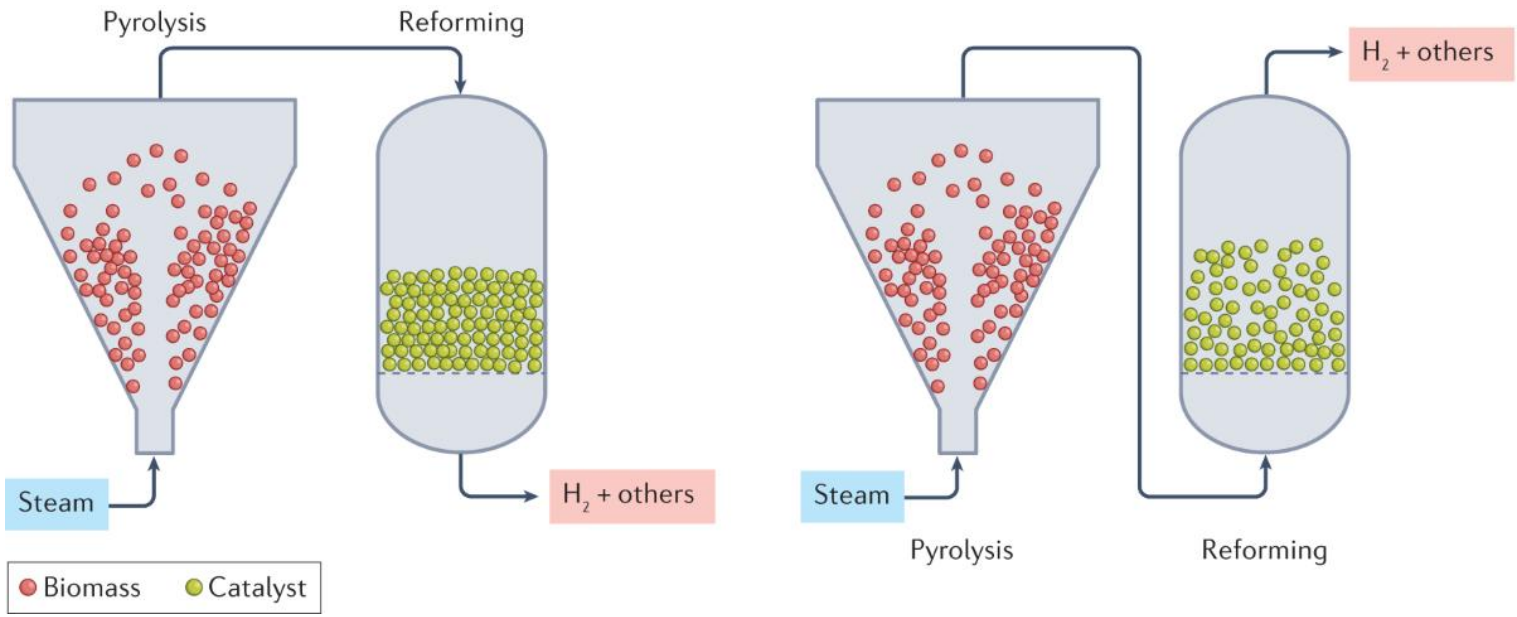
Biohydrogen

❑ Thermochemical Process (Biomass Gasification)

A technology pathway that uses a controlled process involving heat, steam, and oxygen to convert biomass to hydrogen and other products at high temperature (>700 °C), without combustion

- (Step 1) Pyrolysis of biomass to volatiles
- (Step 2) $C_nH_mO_k + (n–k)H_2O \rightarrow nCO + (n+0.5m–k)H_2$
- Subsequently, water–gas shift reaction occurs ($CO + H_2O \rightarrow CO_2 + H_2$ ($\Delta H° = –41.2$ kJ mol^{-1}))



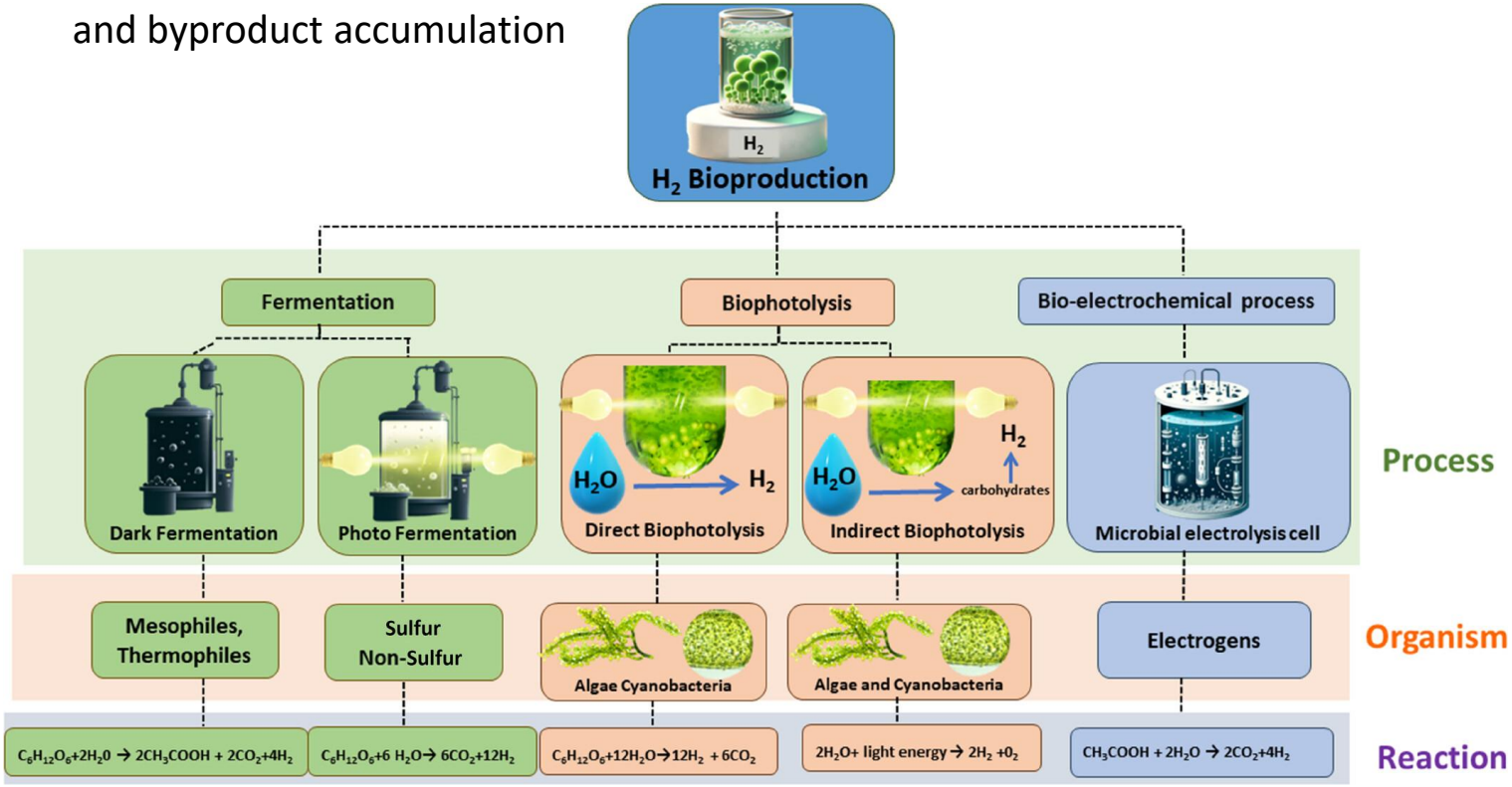
Nat. Rev. Methods Primers, **2** (2022) 20

Biohydrogen

❑ Biological Process

Biologically produced H_2 using microorganisms or biological catalysts (bacteria, microalgae, enzymes)

- Utilizes renewable organic waste and biomass at low temperatures/pressures, enabling a zero/carbon-negative footprint
- Low conversion eff. and slow production speeds due to limited thermodynamic boundaries and byproduct accumulation



Wiley Interdiscip. Rev.: Energy Environ., **13**(3) (2024) e526

Assignment (~08th Sep)

❑ Why Is Hydrogen So Scarce in Earth's Atmosphere?

H_2 makes up only about 0.55 ppm of Earth's atmosphere (See Slide #11). Even though Earth is known as the "water planet," atmospheric H_2 is extremely scarce. A common explanation often states:
"Because H_2 is the lightest molecule, it continually rises through the atmosphere due to buoyancy and eventually escapes into outer space."
Is this explanation physically accurate? If not, what is the correct scientific mechanism behind the low concentration and escape of H_2 from Earth's atmosphere?

(Hint 1)
A helium balloon floats because surrounding air pushes it up. But what happens to a balloon when there is no air left to push it? Can "buoyancy" kick something entirely out into space?

(Hint 2)
Below 100 km, the Earth's atmosphere is constantly stirred by strong winds and turbulence. Does H_2 really rise to the top by itself?

(Hint 3)
Consider the Maxwell–Boltzmann distribution for root-mean-square speed ($v_{rms} = 3k_bT/m)^{0.5}$ vs. Earth's escape velocity v_{esc} = 11.2 km s^{-1} (k_b: Boltzmann constant, T: Temperature, m: mass)

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