

Combined select slides on energy

Prof. S. Sivaram, Prof. S. Sengupta

Amitava Das

CH5106

CHALLENGES TO SUSTAINABILITY

- ✓ Population and earth's carrying capacity (> 9 billion by 2030)
- ✓ Irreversible changes in global climate (+2-3°F 
- ✓ Depletion of earth resources (excessive consumption of natural capital and rapid urbanization)
- ✓ **Access to affordable clean energy (social and quality of life inequities)**

Current World Population

8,252,363,685

[view all people on 1 page >](#)

TODAY

Births today
161,429

Deaths today
76,066

Population Growth today
85,363

THIS YEAR

Births this year
104,273,273

Deaths this year
49,134,055

Population Growth this year
55,139,218

@10.41 AM: 15-10-2025

[https://www.worldometers.info/
world-population/](https://www.worldometers.info/world-population/)

WORLD POPULATION SECTIONS

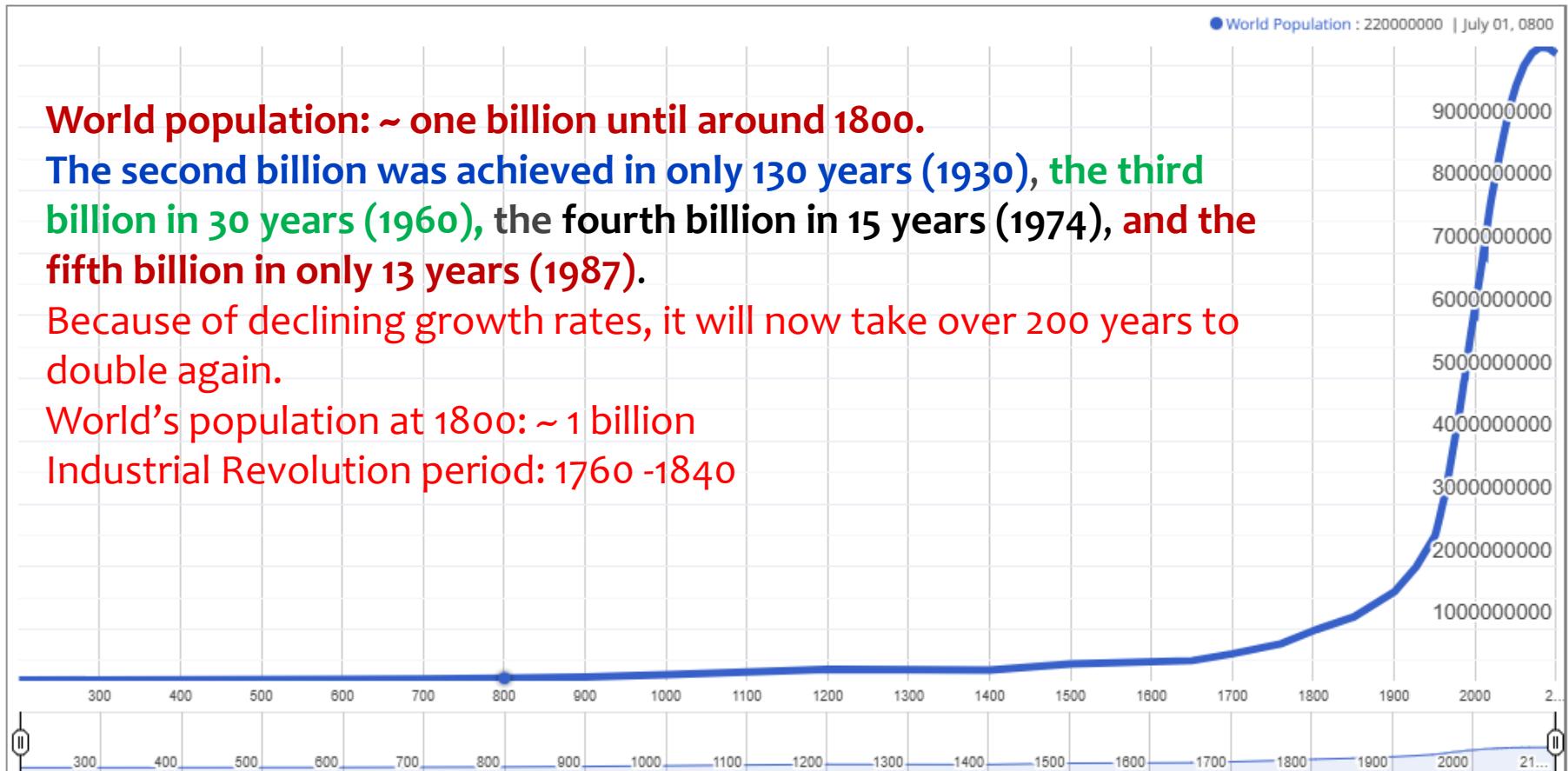
The January–September global surface temperature: Warmest in the 175-year record at 1.28°C above the 1901–2000 average of 14.1°C. National Centres for Environmental Information data indicates a 99.8% chance that 2024 will rank as the warmest year on record. In the best-case scenario, with all policies in place/implemented, the global temperature is still expected to rise by 1.8 °C compared to the pre-industrial average.

Statista: <https://www.statista.com/statistics/1278800/global-temperature-increase-by-scenario/> and <https://www.ncei.noaa.gov/access/monitoring/monthly-report>.

World Population: Past, Present, and Future

(move and expand the bar at the bottom of the chart to navigate through time)

[back to top ↑](#)

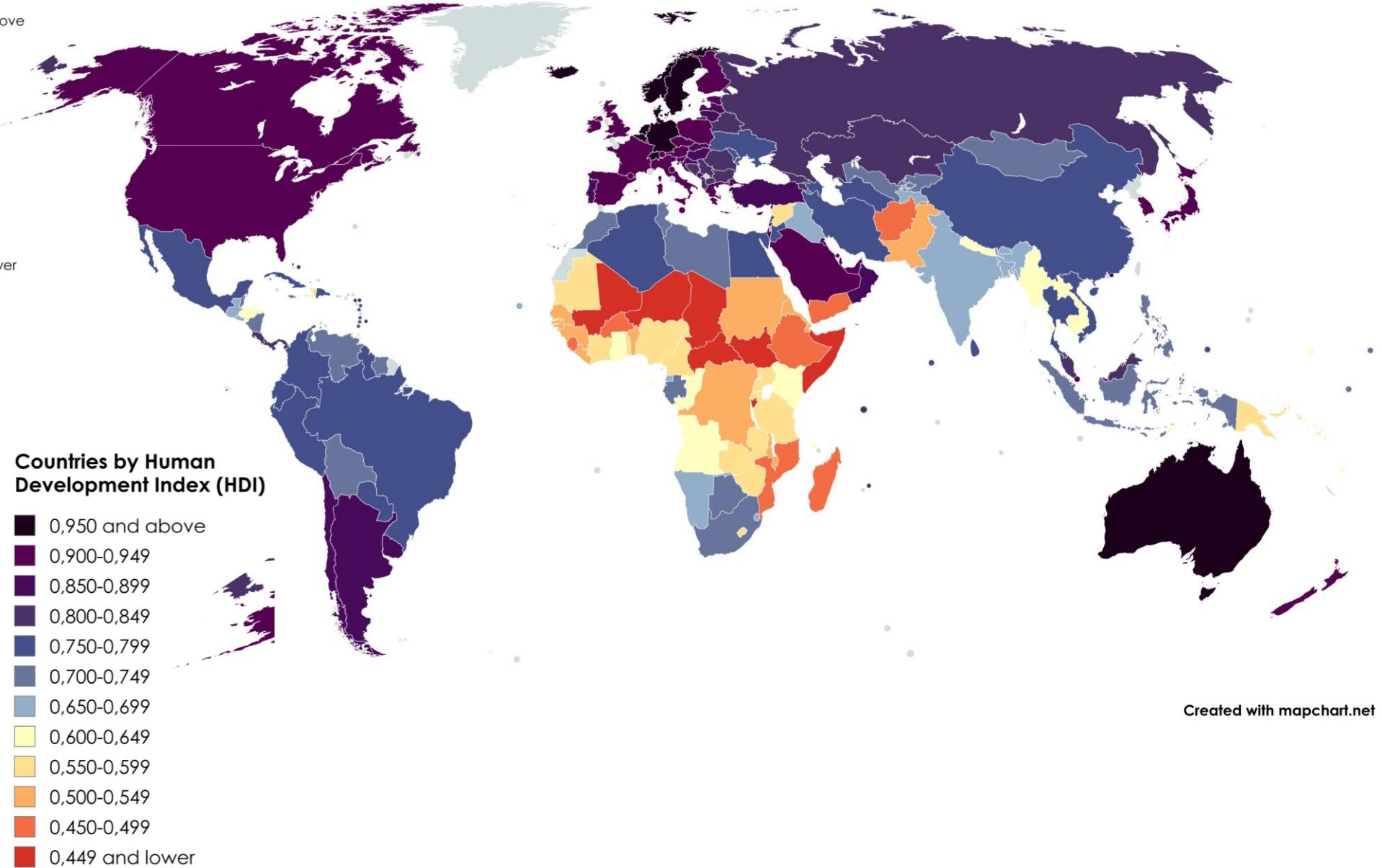


Components of the Human Development Index (HDI)



The Human Development Index, 2025

https://www.reddit.com/r/MapPorn/comments/1kg8cy1/map_of_countries_by_human_development_index_as_of/



The UNDP introduced the Planetary Pressures-adjusted Human Development Index ([PHDI](#)) in the Human Development Report 2020 (UNDP, 2020) and revised it in the 2021/2022 Report (UNDP, 2022). The PHDI adjusts the traditional HDI by factoring in a country's planetary pressures — specifically, its contributions to carbon dioxide (CO₂) emissions and material footprint. It reflects how much a nation's human development depends on environmentally unsustainable practices.

Formula (Simplified)

$$\text{PHDI} = \text{HDI} \times (1 - A)$$

A = adjustment factor based on CO₂ emissions per capita and material footprint per capita

Sustainability: Science, Practice and Policy, 21(1).
<https://doi.org/10.1080/15487733.2025.2454062>

The environmental pressures-adjusted Human Development Index ([eHDI](#)) modifies the HDI by accounting for the ecological and environmental pressures exerted by a country's development model—such as carbon emissions, material footprint, or energy consumption—to provide a more sustainable and holistic measure of progress.

The eHDI adjusts HDI values downward when development is achieved through unsustainable resource use or high environmental degradation.

Thus, it highlights the trade-off between human well-being and ecological sustainability.

Formula (Conceptually)

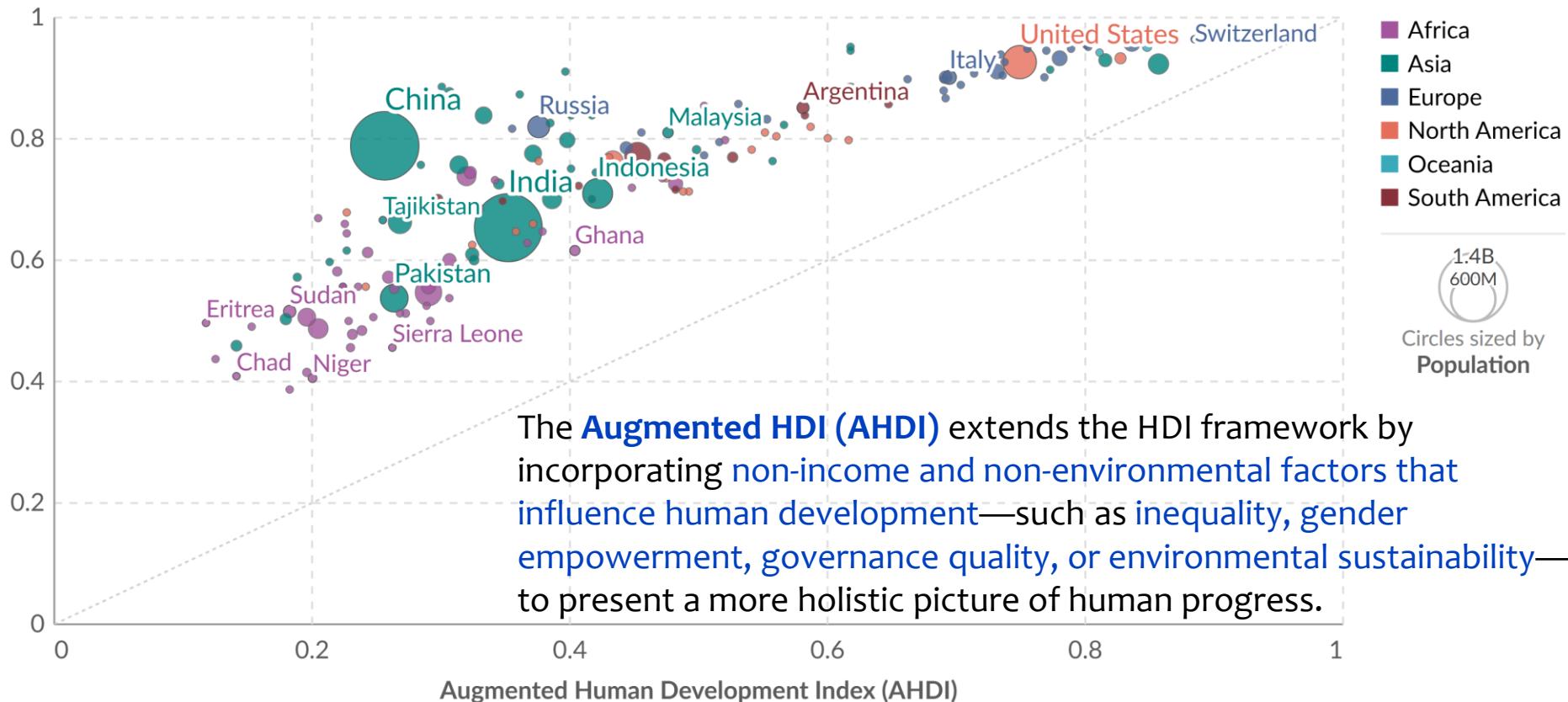
$$\text{eHDI} = \text{HDI} \times (1 - \text{Environmental Pressure Index})$$

Ecological Indicators, 2023, 149, 110181

Human Development Index vs. Augmented Human Development Index, 2020

The Human Development Index (HDI) is a summary measure of key dimensions of human development: a long and healthy life, a good education, and a decent standard of living. The Augmented Human Development Index (AHDI) includes a fourth dimension related to civil and political freedom.

Human Development Index



Data source: UNDP, Human Development Report (2025); Leandro Prados de la Escosura (2021)

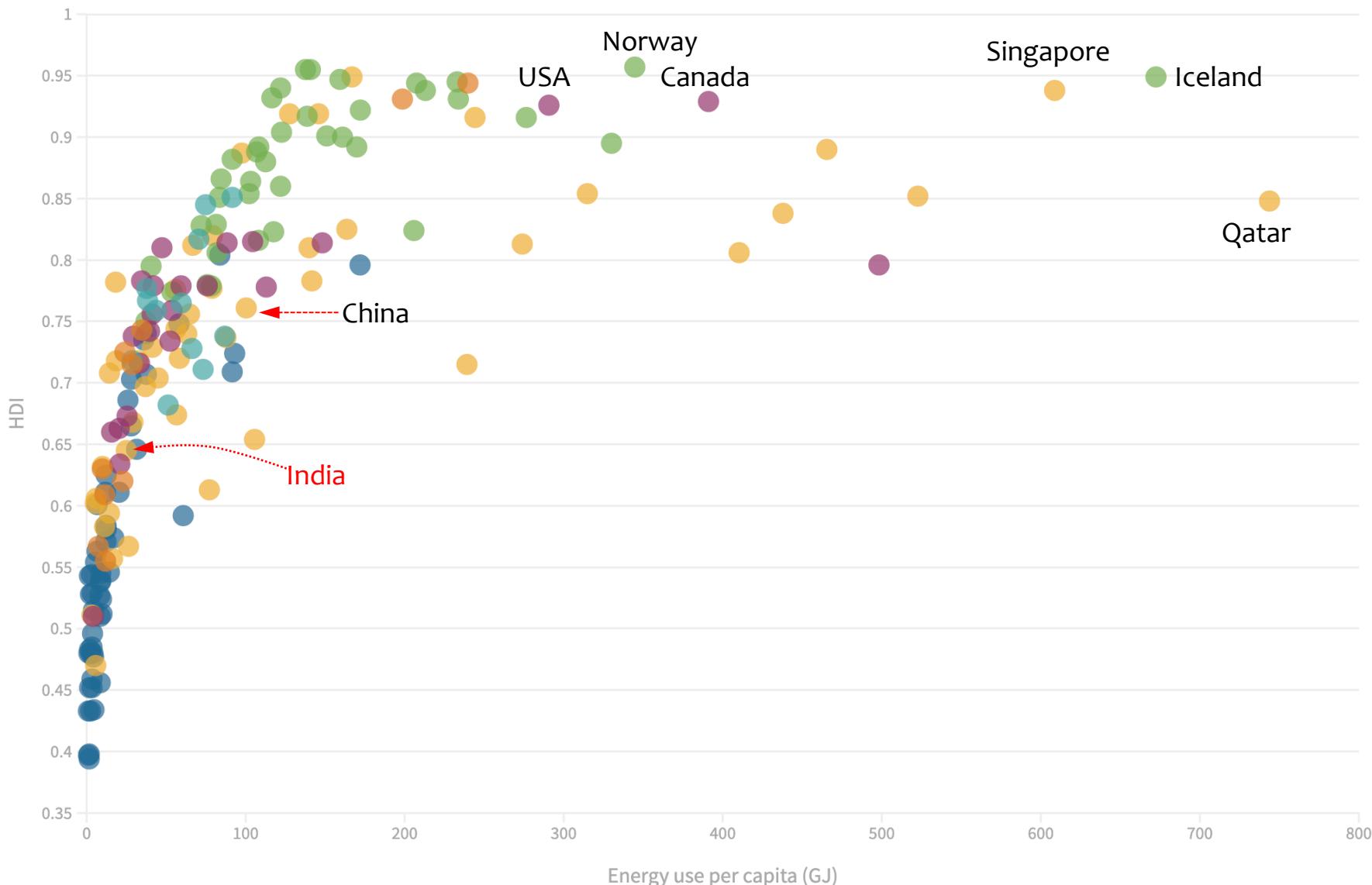
OurWorldinData.org/human-development-index | CC BY

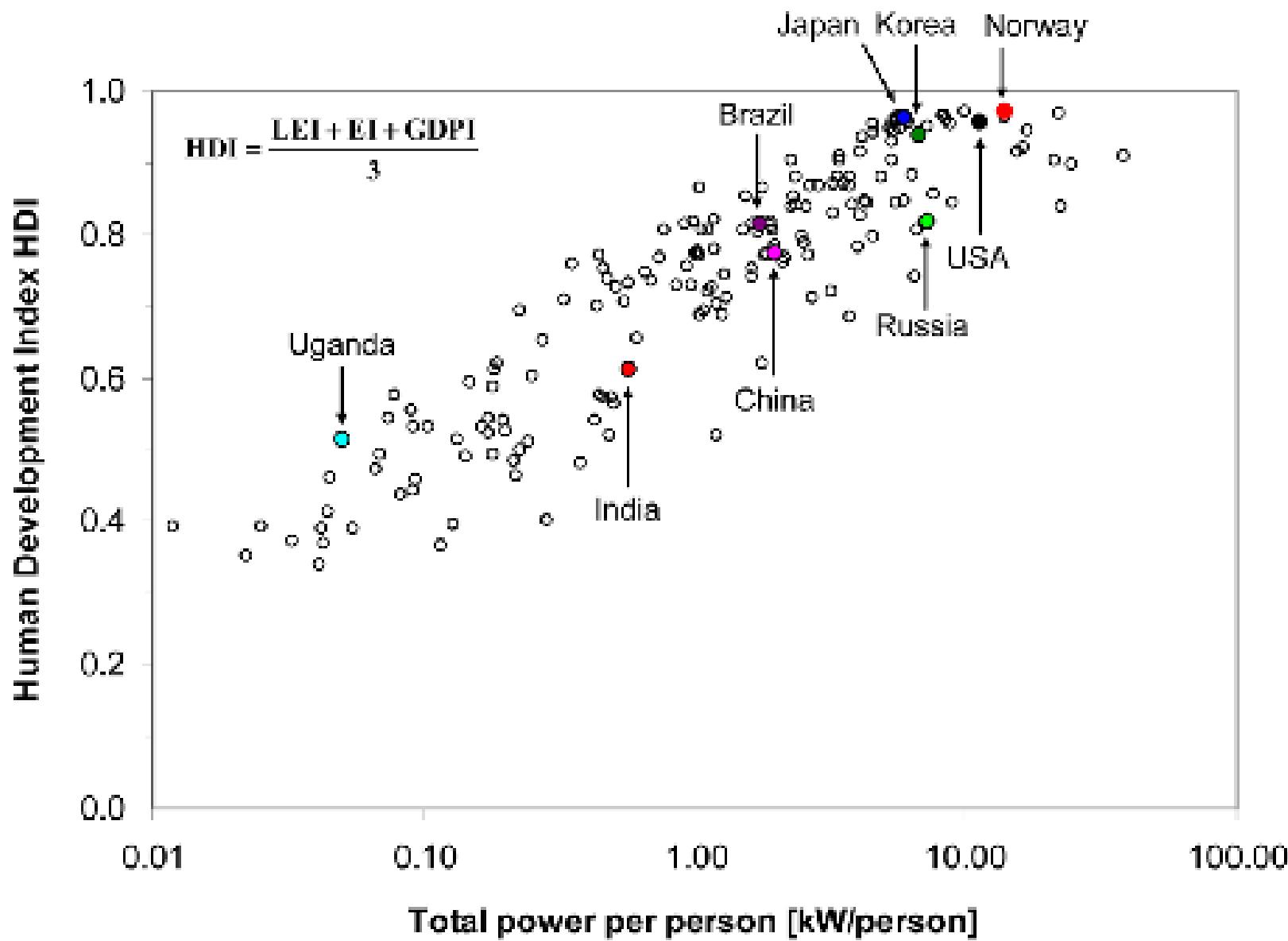
Data source: UNDP, Human Development Report (2025); Leandro Prados de la Escosura (2021) – Learn more about this data

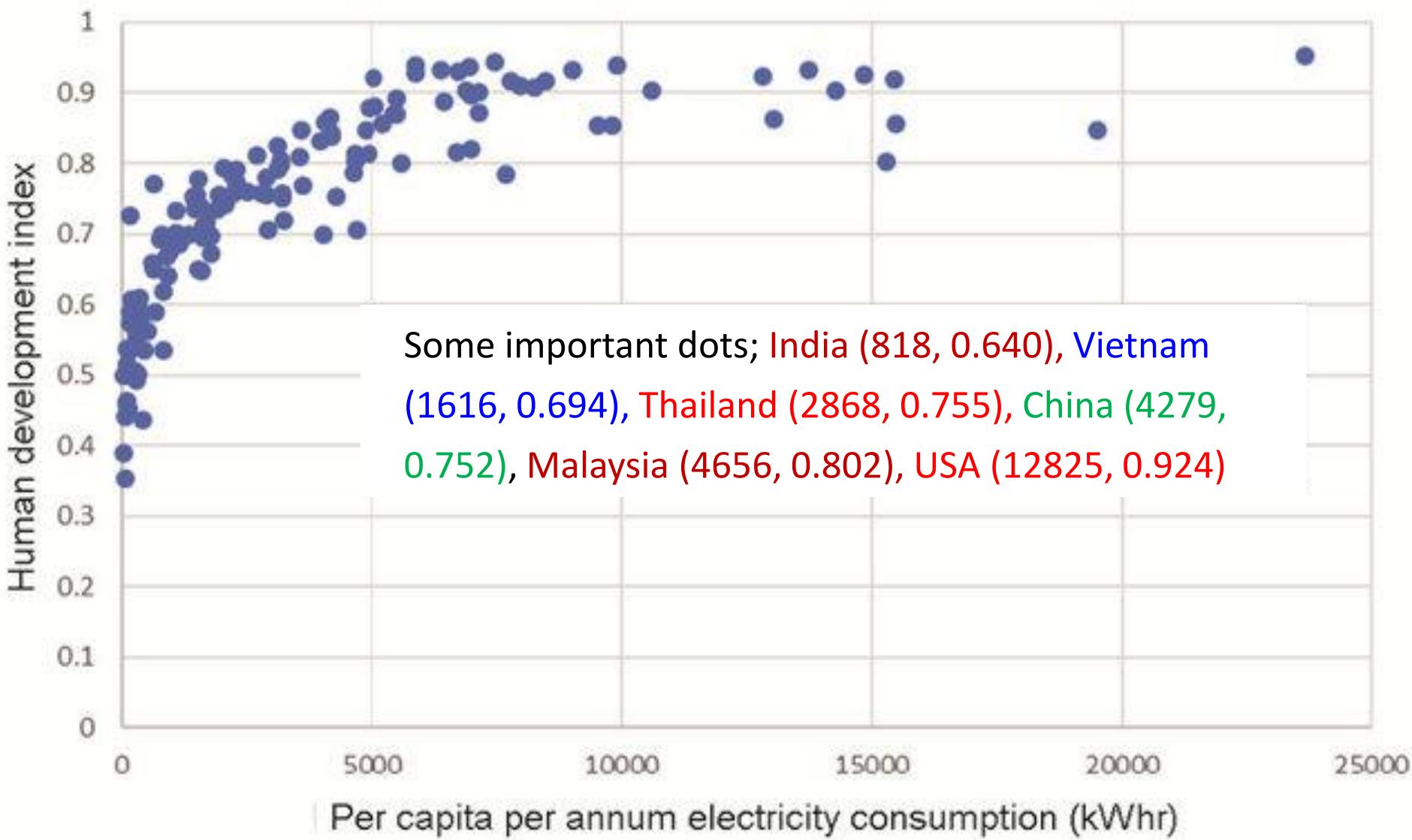
The Human Development Index (HDI) and energy use per capita, 2019

The HDI is a 0 to 1 composite index based on indicators for health, education, and income.

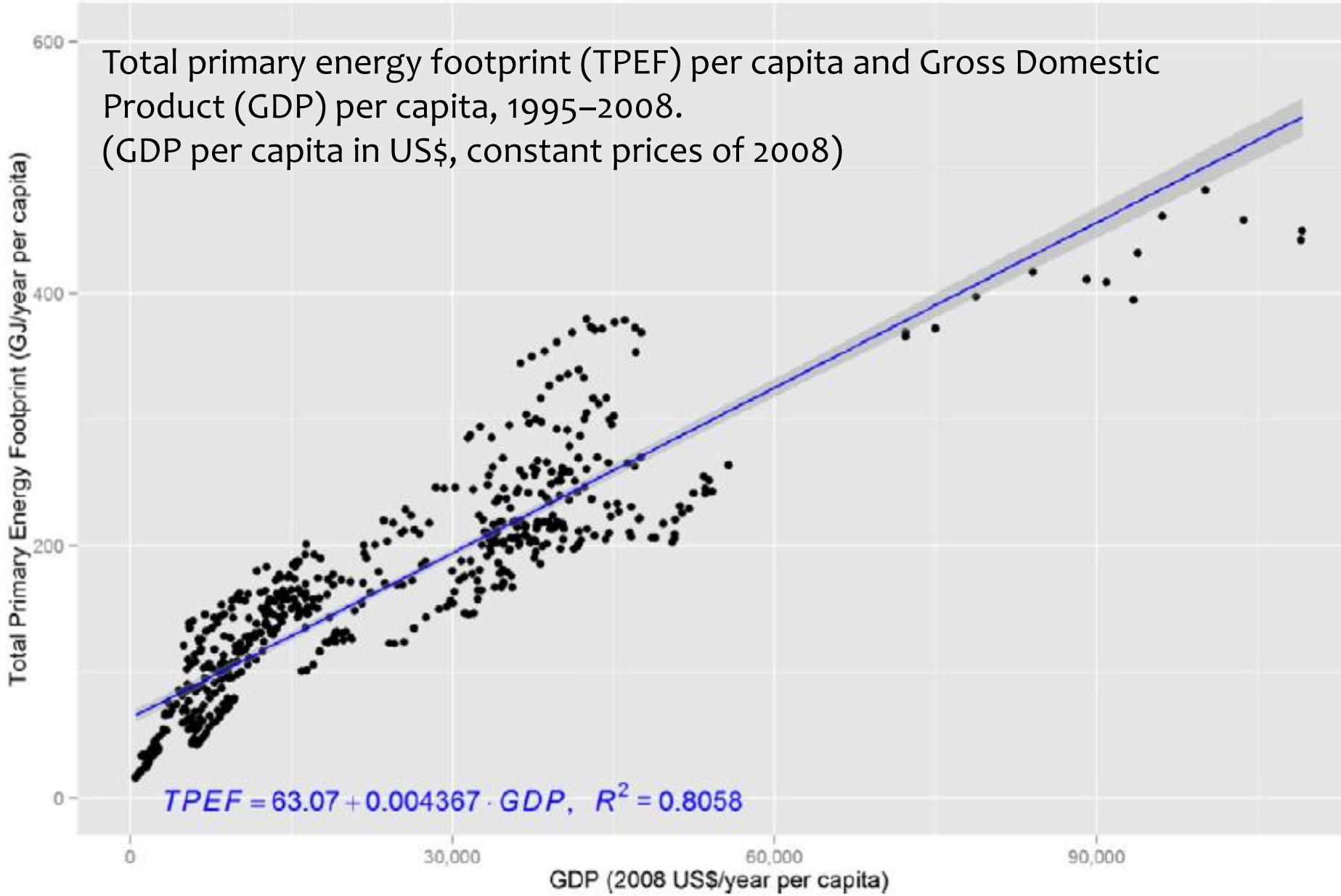
Continent ● Africa ● Asia ● Europe ● North America ● South America ● Oceania







- ✓ R. Grover, Current Science, 2020, 119, 25
- ✓ Data for electricity consumption: Key World Energy Statistics, International Energy Agency, 2018
- ✓ Human Development Index: Human Development Indices and Indicators, Statistical Update, United Nations Development Programm, 2018



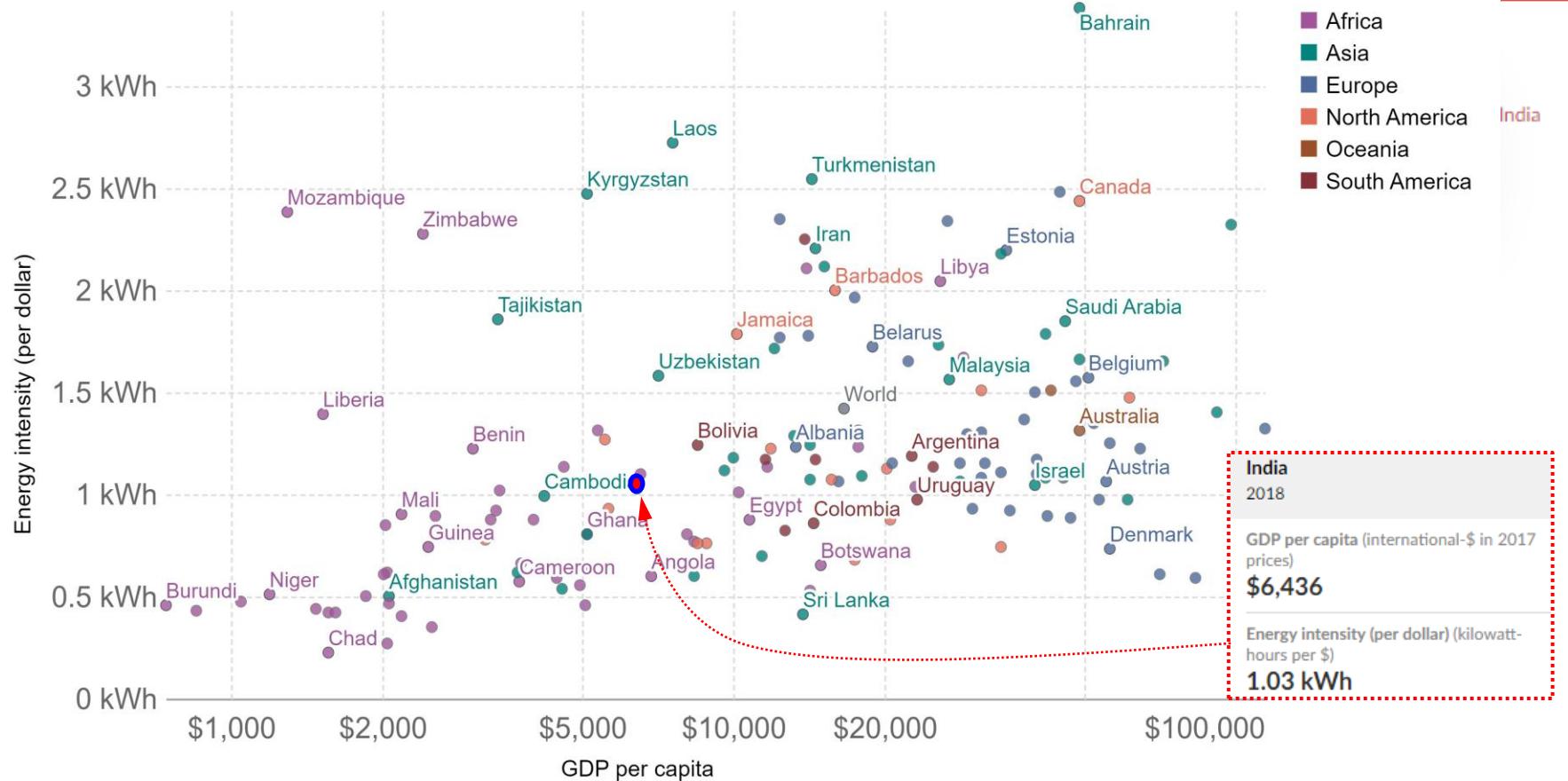
Alternate model: Energy-environmental Kuznets curve

Energy intensity vs. GDP per capita, 2018

Energy intensity represents energy consumption per unit of GDP – it's measured in kilowatt-hours per international-\$.

Ene
Energy

+ Ad

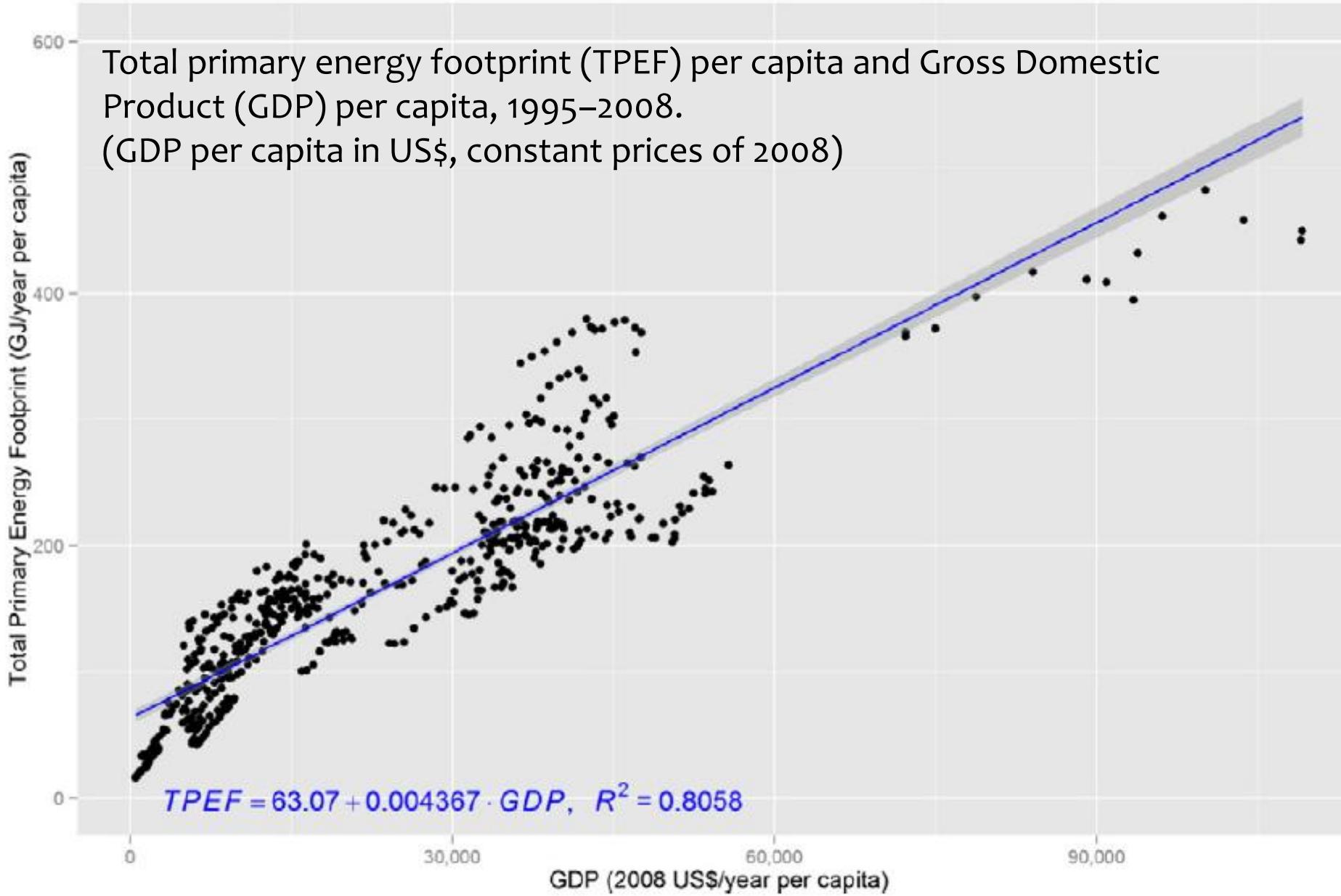


Source: U.S. Energy Information Administration (EIA); Energy Institute Statistical Review of World Energy (2023), Data compiled from multiple sources by World Bank

Note: GDP per capita is measured in constant international-\$¹ which corrects for inflation and cross-country price differences.

OurWorldInData.org/energy • CC BY

1. International dollars: International dollars are a hypothetical currency that is used to make meaningful comparisons of monetary indicators of living standards. Figures expressed in international dollars are adjusted for inflation within countries over time, and for differences in the cost of living between countries. The goal of such adjustments is to provide a unit whose purchasing power is held fixed over time and across countries, such that one international dollar can buy the same quantity and quality of goods and services no matter where or when it is spent. Read more in our article: What are Purchasing Power Parity adjustments and why do we need them?



Alternate model: Energy-environmental Kuznets curve

Table 8.2: Per-Capita Energy Consumption and Energy Intensity

Govt, Ministry of Statistics and Program Implementation National Statistical Office <https://www.mospi.gov.in/>

Year	Energy Consumption in petajoules	Mid year population (in Thousands) *	GDP at 2011-12 prices (Rs. crore) **	Per Capita Energy Consumption (in Megajoules)	Energy Intensity (Megajoules per rupee)
2011-12	24,121	12,20,171	87,36,329	19,769	0.2761
2012-13	25,805	12,36,220	92,13,017	20,874	0.2801
2013-14	26,302	12,52,267	98,01,370	21,003	0.2683
2014-15	27,841	12,68,310	1,05,27,674	21,951	0.2645
2015-16	28,665	12,84,350	1,13,69,493	22,319	0.2521
2016-17	29,556	12,99,434	1,23,08,193	22,745	0.2401
2017-18	31,153	13,13,815	1,31,44,582	23,712	0.2370
2018-19	32,805	13,28,206	1,39,92,914	24,699	0.2344
2019-20	32,729	13,42,586	1,45,34,641	24,378	0.2252
2020-21	30,354	13,56,980	1,36,87,118	22,369	0.2218
2021-22 (P)	33,508	13,70,311	1,49,25,840	24,453	0.2245
Growth rate of 2021-22 (P) over 2020-21(%)	10.39	0.98	9.05	9.32	1.23
CAGR 2012-13 to 2021-22 (P) (%)	2.94	1.15	5.51	1.77	-2.43

(P): Provisional

Energy Intensity=Amount of energy consumed for producing one unit of Gross Domestic Product.

* Mid-Year (as on 1st October) population has been taken from Population Projections for India and states 2011 – 2036; Report of the Technical Group On Population Projections , July, 2020

** GDP estimates are at base 2011-12 price as per the National Accounts Division's, NSO, MoSPI.

Table 8.2: Per-Capita Energy Consumption and Energy Intensity

Year	Energy Consumption in petajoules	Mid year population (in Thousands) *	GDP at 2011-12 prices (Rs. crore) **	Per Capita Energy Consumption (in Megajoules)	Energy Intensity (Megajoules per rupee)
2013-14	26,822	12,52,267	98,01,370	21,419	0.2737
2014-15	28,453	12,68,310	1,05,27,674	22,434	0.2703
2015-16	29,063	12,84,350	1,13,69,493	22,629	0.2556
2016-17	29,713	12,99,434	1,23,08,193	22,866	0.2414
2017-18	30,966	13,13,815	1,31,44,582	23,569	0.2356
2018-19	32,712	13,28,206	1,39,92,914	24,629	0.2338
2019-20	32,548	13,42,586	1,45,34,641	24,243	0.2239
2020-21	29,807	13,56,980	1,36,94,869	21,965	0.2176
2021-22	33,018	13,70,311	1,50,21,846	24,095	0.2198
2022-23(P)	35,159	13,82,894	1,60,71,429	25,424	0.2188
Growth rate of 2022-23 over 2021-22 (%)	6.48	0.92	6.99	5.52	-0.47
CAGR 2013-14 to 2022-23 (P) (%)	3.05	1.11	5.65	1.92	-2.46

P: Provisional

Energy Intensity=Amount of energy consumed for producing one unit of Gross Domestic Product.

* Mid-Year (as on 1st October) population has been taken from Population Projections for India and states 2011 – 2036; Report of the Technical Group On Population Projections, July, 2020

** GDP estimates are at base 2011-12 price as per the National Accounts Divisions's, NSO, MoSPI.

CO₂ emissions per capita vs GDP per capita

Per capita consumption-based CO₂ emissions

20 t

15 t

10 t

5 t

2.5 t

0 t

CO₂ emissions
are too high

Energy poverty

\$2,000 \$5,000 \$10,000 \$20,000 \$50,000 \$100,000

GDP per capita (int.-\$)

To end climate change the long-run goal is that net-emissions decline to zero.

Data for 2017: Global Carbon Project, UN Population, and World Bank.

OurWorldInData.org – Research and data to make progress against the world's largest problems.

Licensed under CC-BY by the author Max Roser.

Our challenge: find large-scale energy alternatives to fossil fuels that are affordable, safe and sustainable

Energy as a Human Right:

Electricity consumption is closely and positively related to global economic and HDI across different geographical, social, and cultural contexts. The seventh goal (SDG 7) aims to ensure access to affordable, reliable, sustainable, and modern energy for all. Despite these, access to electricity is not explicitly recognized as a universal human right.

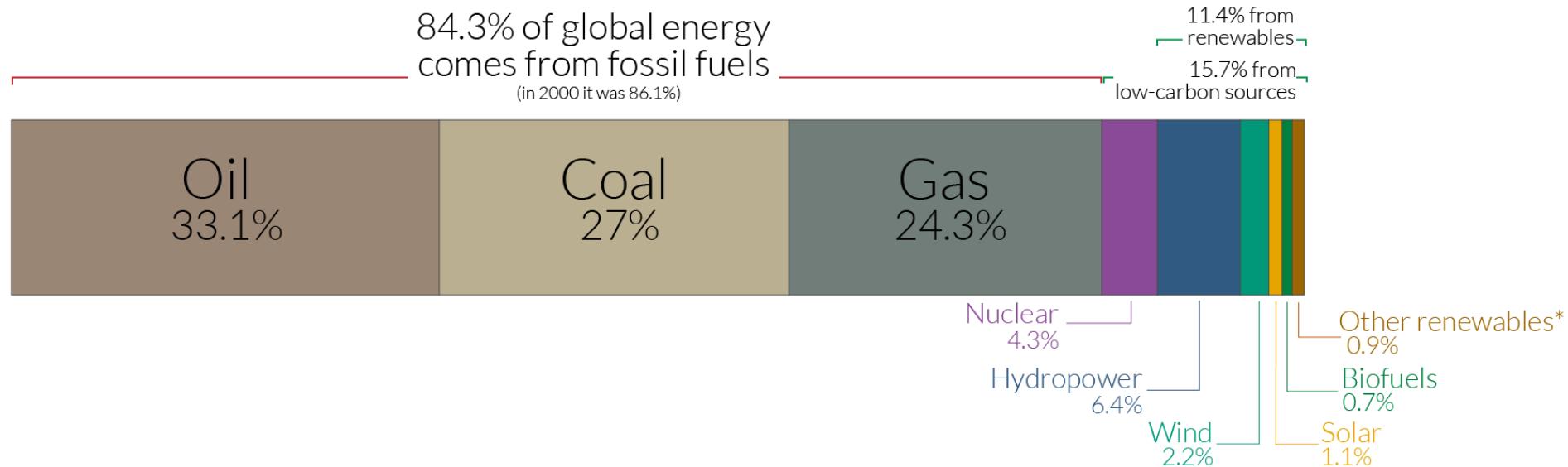
While not legally binding, the 17 goals of SDGs have multiple links to human rights law and explicitly ‘seek to realize the human rights of all’. Access to energy is not codified in human rights law (like the right to life, for example), it can be a prerequisite for the enjoyment of other human rights (such as the right to life, among other rights). It is a derivative human right entirely reliant on its links with existing human rights obligations enshrined in international human rights law.

Energy consumption by source, World

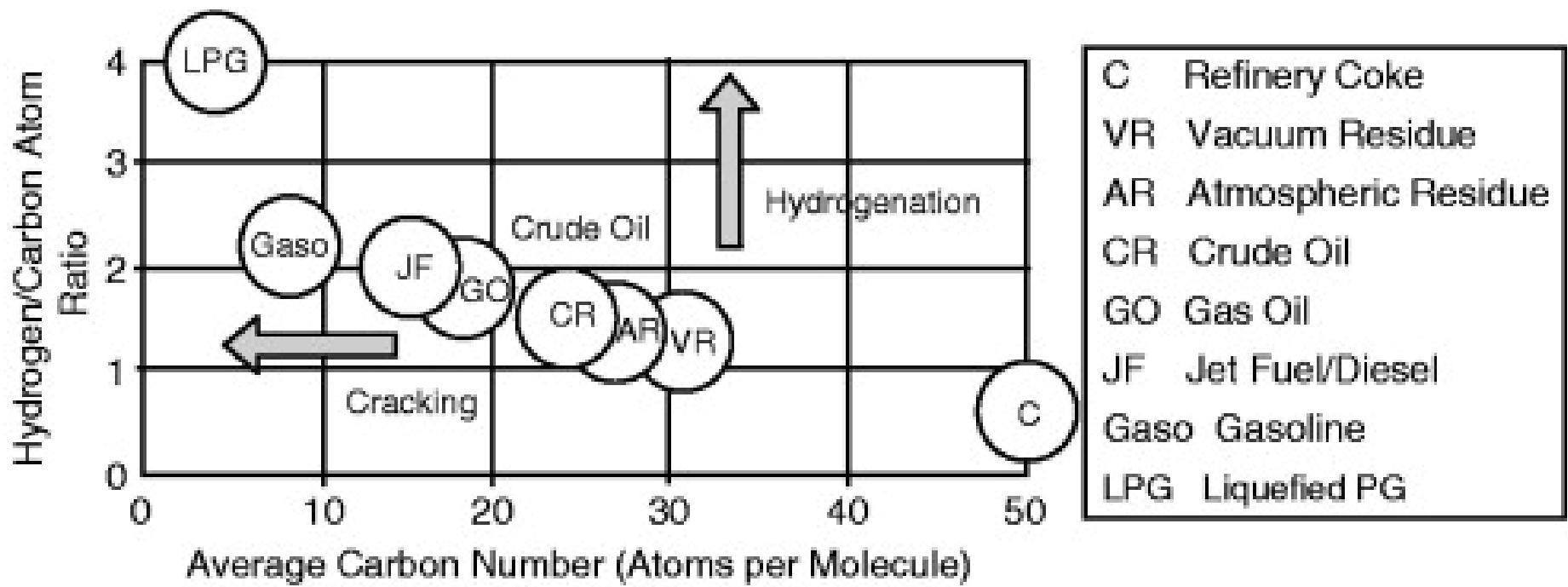
Primary energy consumption is measured in terawatt-hours (TWh). Here an inefficiency factor (the 'substitution' method) has been applied for fossil fuels, meaning the shares by each energy source give a better approximation of final energy consumption.

Global primary energy consumption by source

The breakdown of primary energy is shown based on the 'substitution' method which takes account of inefficiencies in energy production from fossil fuels. This is based on global energy for 2019.



*'Other renewables' includes geothermal, biomass, wave and tidal. It does not include traditional biomass which can be a key energy source in lower income settings.



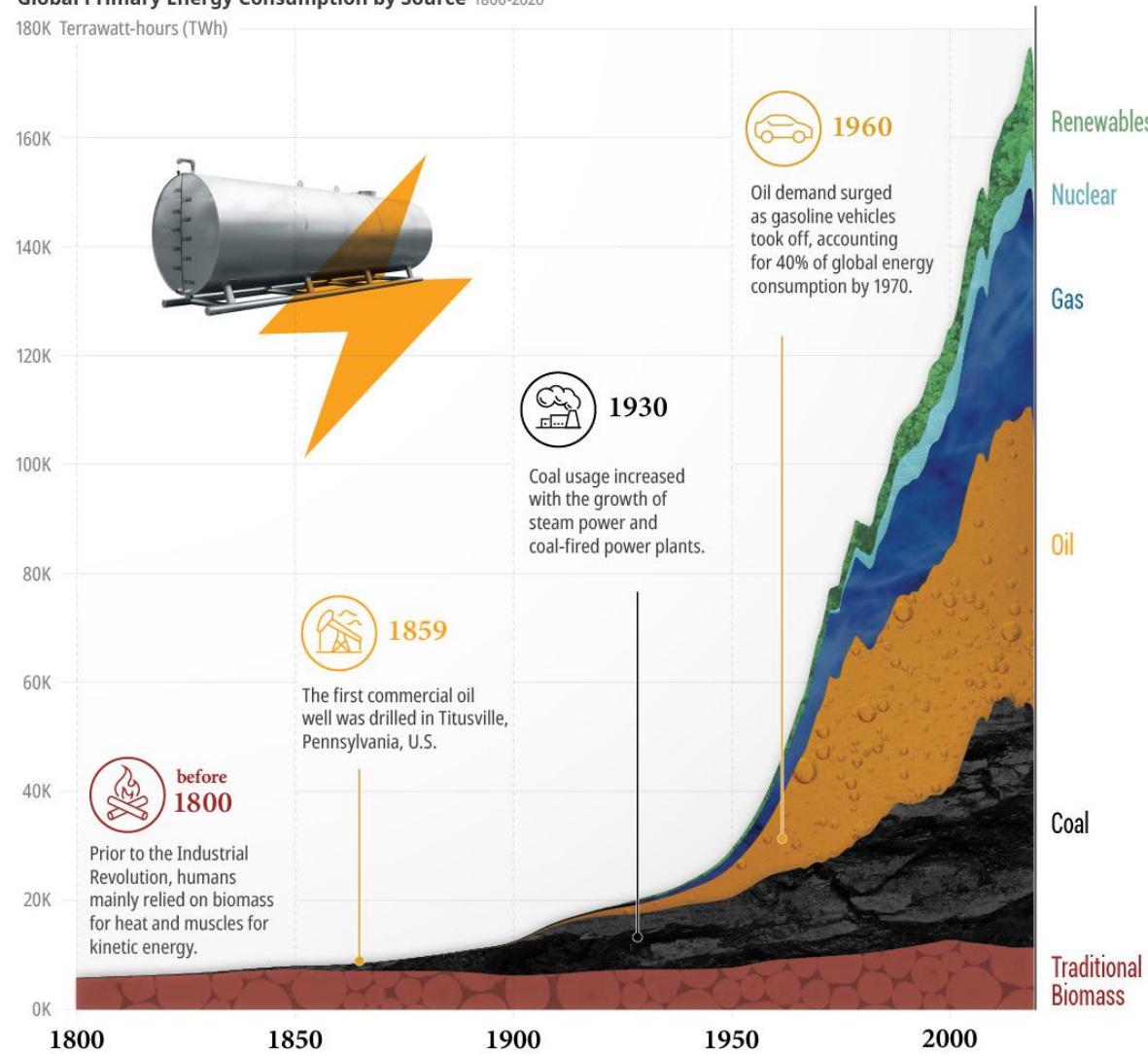
THE HISTORY OF Energy Transitions

The economic and technological advances over the last 200 years have transformed how we produce and consume energy.

Here's how the global energy mix has evolved since 1800.

Global Primary Energy Consumption by Source 1800-2020

180K Terrawatt-hours (TWh)



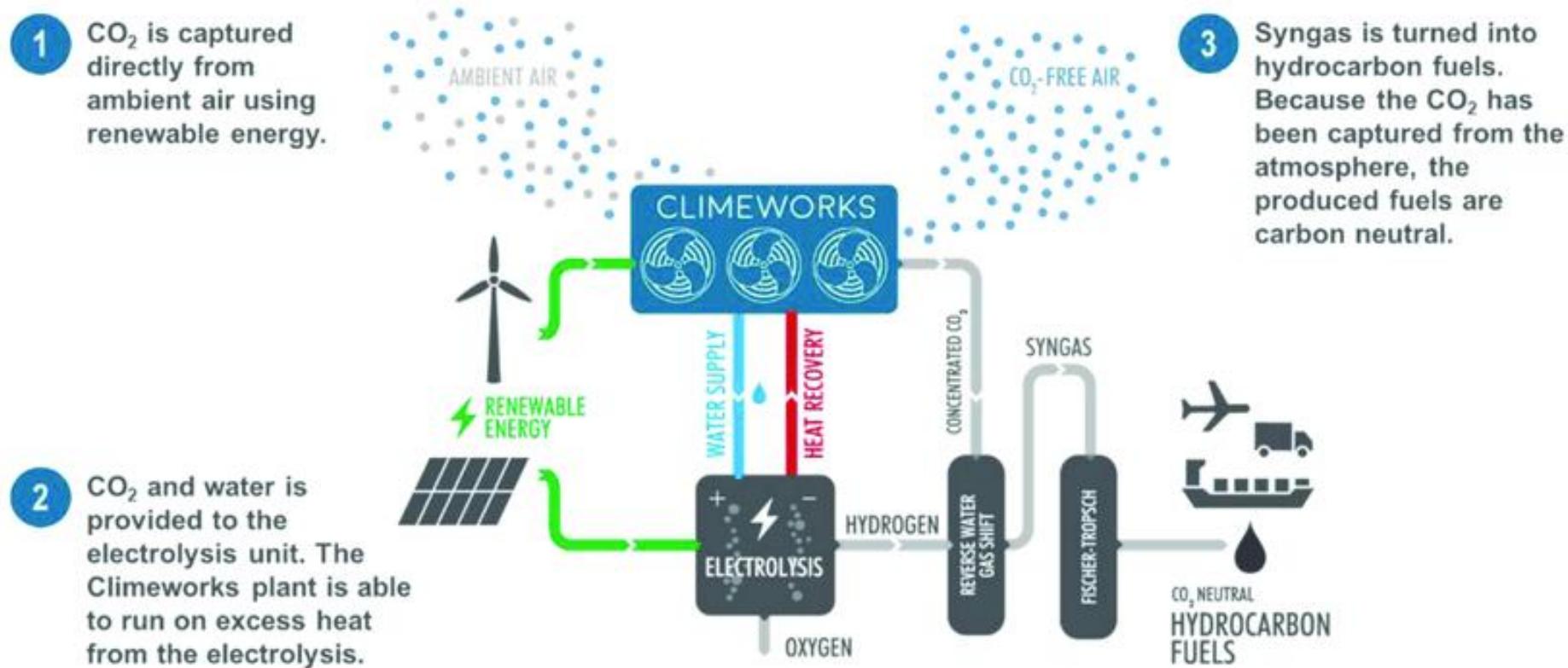
Demand and technological innovations are the biggest drivers of these shifts, and they are playing a key role in the current move towards cleaner energy.

- Coal as fuel contributes to ~ 50% of the electricity generation in India. Coal is more abundant than oil and coal reserves are far more abundant than oil reserves in this world.
- Coal burning enhances the CO₂ footprint. Burning coal results in NOx and SOx, heavy metals (such as Hg), and radioactive metals, which need to be cleaned. Apart from these coal burning adds to a significant amount of ash.
- This is why we need clean coal technology.

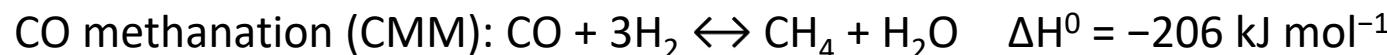
Mercury in coal is released to flue gases in the form of Hg⁰ during combustion in a thermal power plant. Decreasing temperature from over 800°C to below 300°C in flue gases leaving boilers or furnaces promotes oxidation of Hg⁰ to gaseous Hg²⁺, with a portion of Hg²⁺ adsorbed onto fly ash to form particulate-bound mercury (Hg_p)

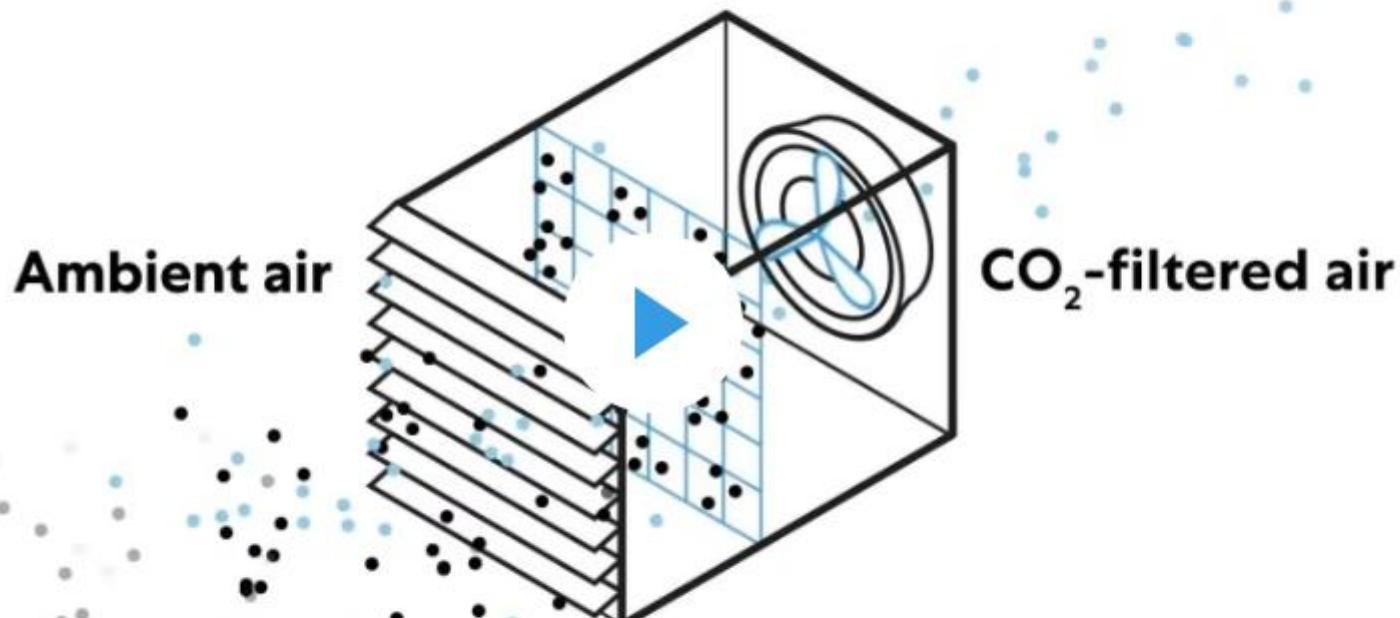
The overall trend is not on track with the Net Zero Emissions by 2050 Scenario, which calls for immediate reductions and a global decline in unabated coal-fired generation of around 55% by 2030 compared to 2022 levels, and a complete phase-out by 2040. About 70% of world steel production depends on coal feedstock. Coal is the world's most abundant and widely distributed fossil fuel source.

The world's first commercial plant for direct air capture of CO₂ is located in Hinwil, Switzerland @ 2017. In recent years Direct Air Capture (DAC) has established itself as a promising approach to atmospheric Carbon Dioxide Removal (CDR) also referred to as Negative Emissions.



Reverse water gas shift (RWGS)





The air is drawn into a collector with a fan, and CO₂ is captured on the surface of a highly selective filter material that sits inside the collector.

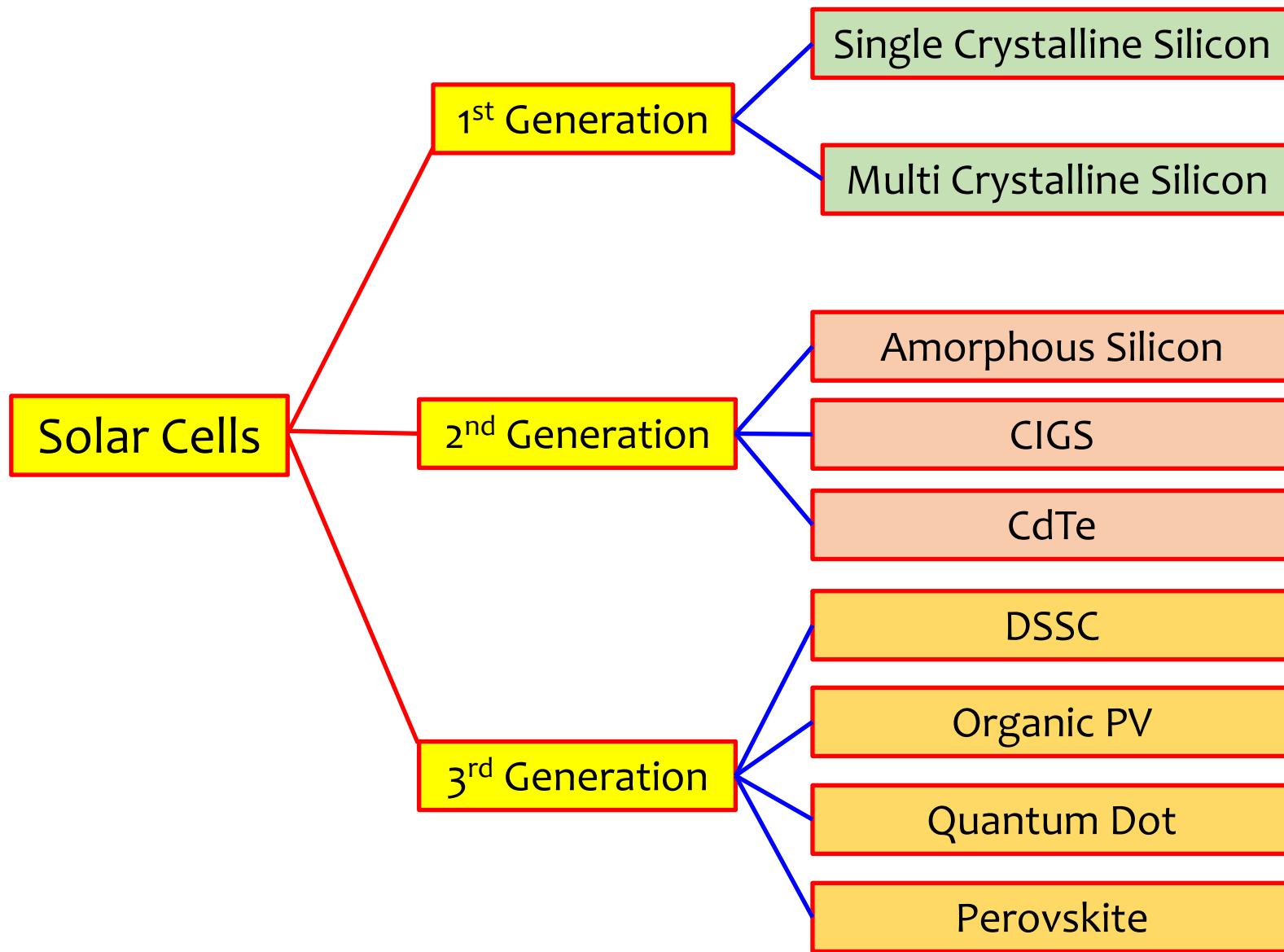
Third Generation Solar Cells

DSSC

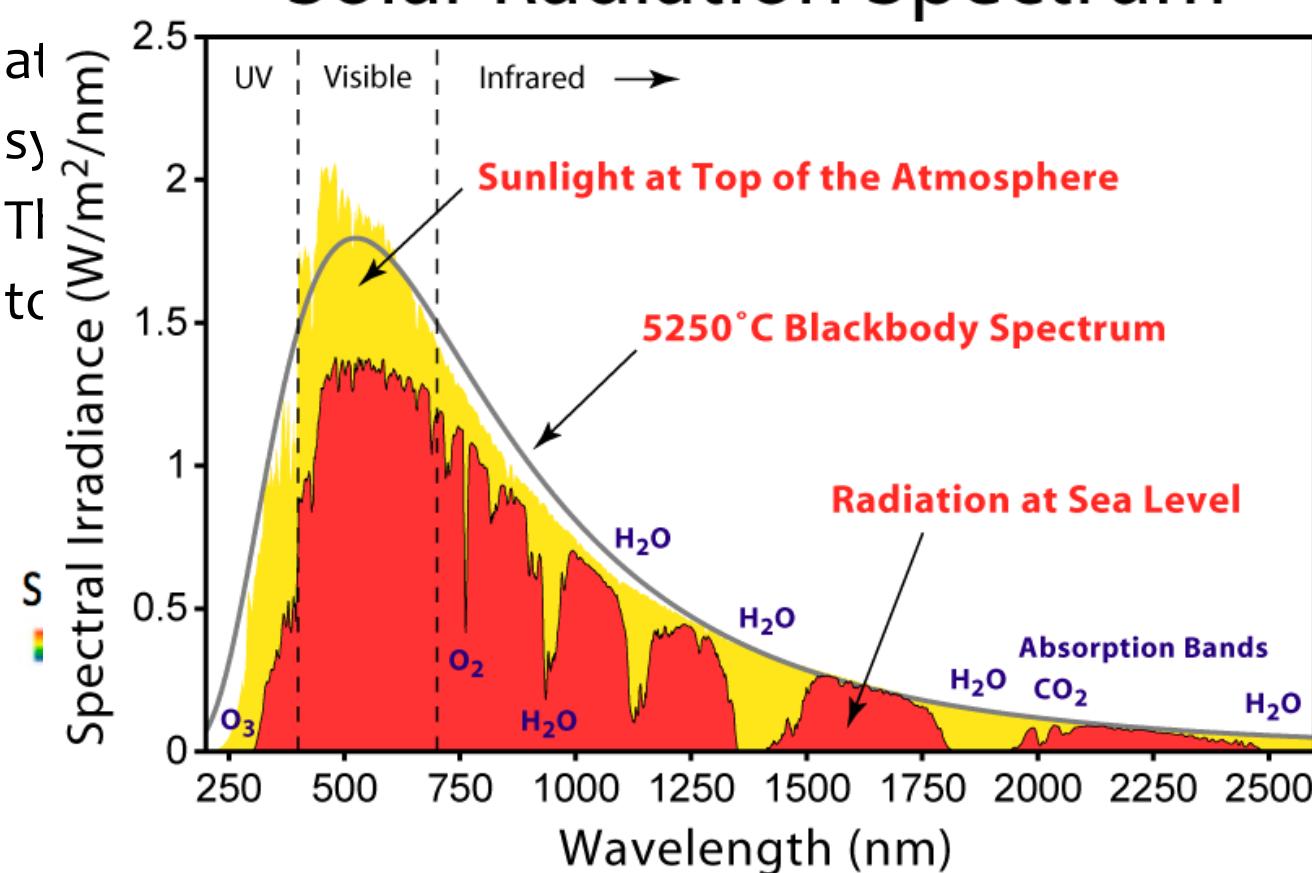
Prof. S. Sivaram
Prof. S. Sengupta
[Amitava Das](#)

[CH5106](#)

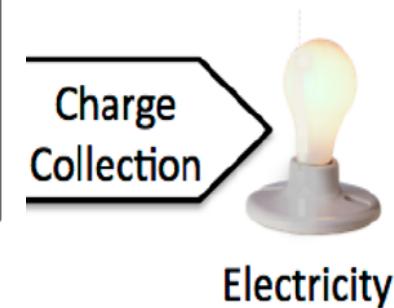
Solar Cell Developments—Three Generations



Solar Radiation Spectrum



it on the Earth's
orbited by the Earth
atmosphere itself.
in a day is sufficient



Solar irradiance spectrum above the Earth's atmosphere and at the
surface. Date source: www.nrel.gov. How does light into electricity in a typical solar cell

Pure silicon (intrinsic silicon) is a poor semiconductor, not an insulator.

- Band gap: Silicon has a moderate band gap of ~ 1.12 eV at room temperature — large enough that few electrons are thermally excited to the conduction band, but small enough that some conduction does occur.
- Electrical conductivity: At room temperature, its conductivity is around 10^{-4} to 10^{-6} S/cm, which is much lower than metals but far higher than true insulators (which have conductivities $< 10^{-12}$ S/cm).
- Temperature dependence: As temperature increases, more electrons are thermally excited across the band gap, and conductivity rises sharply — a hallmark of semiconductors.
- At 0°K : Behaves like an insulator (no free charge carriers).
- 300°K : Behaves as a poor (intrinsic) semiconductor.
- Doped with P/B: A good semiconductor (n-type or p-type).

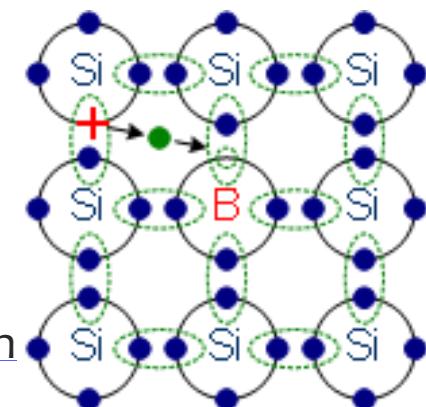
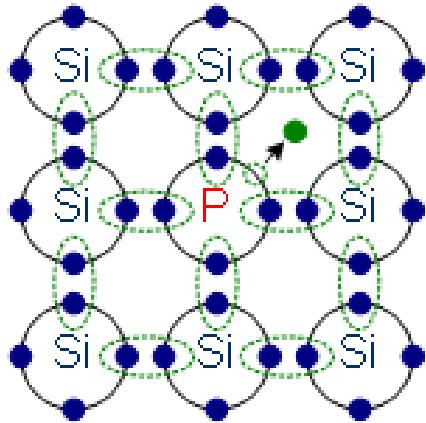
N-Type (Negative)

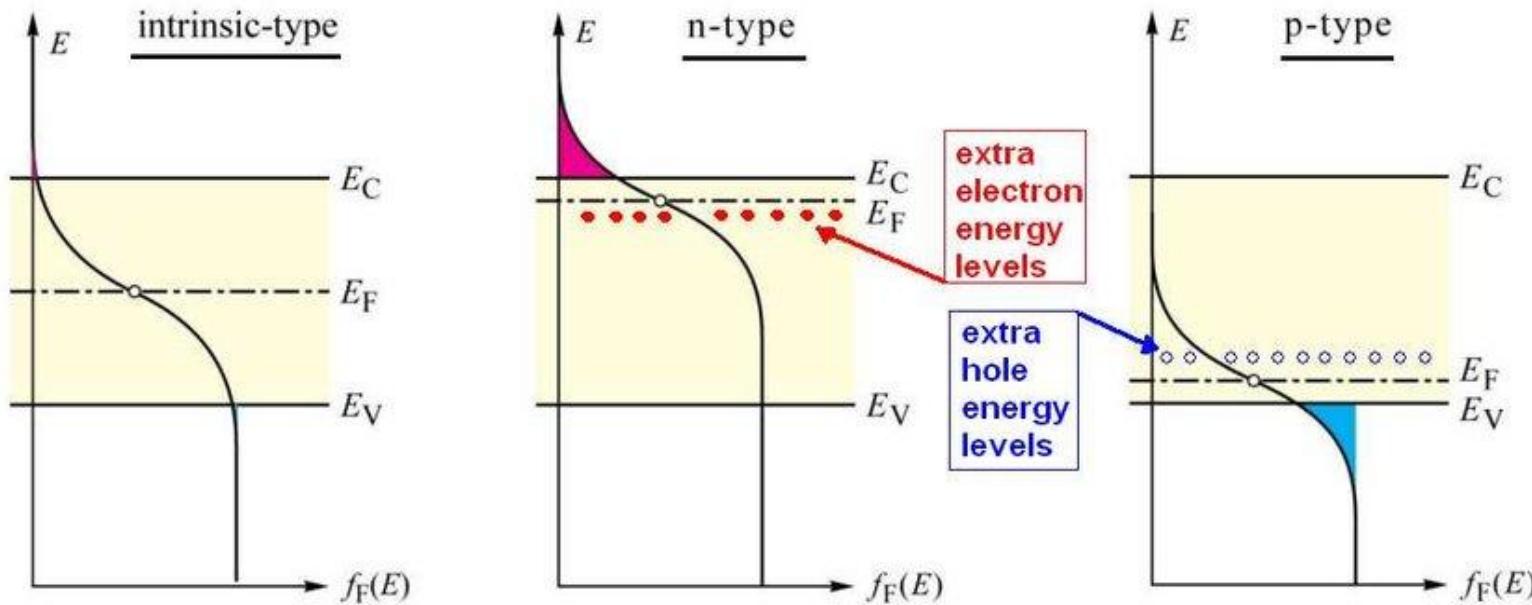
Silicon is doped with phosphorus gas to make it conductive. A silicon atom has four electrons in its outer shell and bonds tightly with four surrounding silicon. However, phosphorus has five electrons, and when combined, the fifth electron becomes a "free" electron that moves easily within the crystal when a voltage is applied. Because the charge carriers are electrons, n-type refers to a negative charge.

P-Type (Positive)

Silicon doped with boron gas that turns it into a conductive material that readily accepts electrons when voltage is applied. Boron has only three electrons in its outer shell and can bond with only three of the four surrounding silicon atoms. This leaves one silicon atom with a vacant location in its outer shell, called a "hole," that readily accepts an electron. Because the charge carriers are holes, p-type silicon is said to have a positive charge.

Pure silicon is a poor conductor. When doped (e.g., with phosphorus for n-type or boron for p-type), the number of charge carriers increases dramatically, and it becomes a good semiconductor.





The Fermi level determines the probability of electron occupancy at different energy levels. The closer the Fermi level is to the conduction band energy, the easier it will be for electrons in the valence band to transition into the conduction band. Electrons settle into the lowest available energy states at absolute zero temperature.

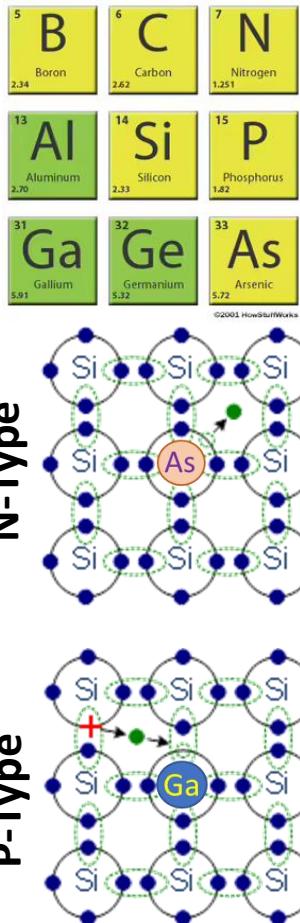
The gap between the valence and conduction bands is called the energy gap. At the Fermi level (when $E=E_f$), the probability simplifies to $\frac{1}{2}$ and thus E_f lies halfway between the valence and conduction band, or in the middle of the energy gap ($E_{\text{gap}}/2$).

Impurities and temperature can affect the Fermi level. Semiconductor atoms are closely grouped together in a crystal lattice and so they have very few free electrons to be good conductors. The ability of semiconductors to conduct electricity can be greatly improved by introducing donor or acceptor atoms to the crystalline structure, either producing more free electrons or more holes. This process is called “doping” and as the semiconductor material is no longer pure, these donor and acceptor atoms are collectively referred to as “impurities”. For both N-type or P-type semiconductors, the position of the Fermi level relative to the band structure can be controlled to a significant degree by doping.

Gallium Arsenide (GaAs): External quantum efficiency (EQE) and reflectance curves of the fabricated GaAs thin-film solar cell. The sudden increase in the spectral response of the EQE around 880 nm corresponds to the band gap energy of GaAs. The high EQE of >80% occurs in the 500–800nm wavelength range.

The GaAs thin-film solar cell is a top contender in the thin-film solar cell market in that it has a high power conversion efficiency (PCE) compared to that of other thin-film solar cells. The efficiency of ~ 28.9%, while this is the most expensive.

Scientific Reports | 6:30107 | DOI: 10.1038/srep30107



The following graph is the famous limit efficiency (%) of Shockley-Queisser for p-n junctions in function of the energy band gap (eV):

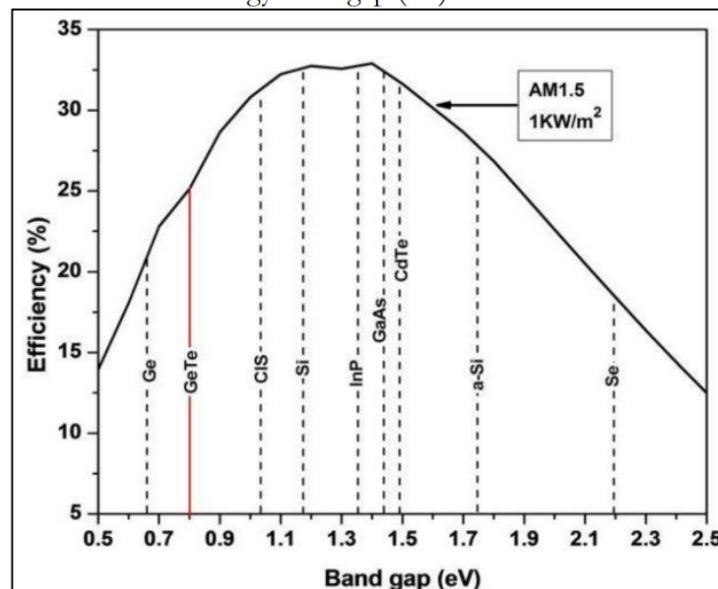


Illustration 6 - S.Q. efficiency limit in function of the energy band gap and the correspondence for different solar cells materials.

The maximum efficiency is reached around 33.7% for a single pn-junction PV cell, assuming AM 1.5 solar spectrum and a temperature of the cell of 300 K and it occurs at a band gap of 1.34eV, which is very close for silicon solar cells, which have a band gap of 1.12eV.

Need
to redo

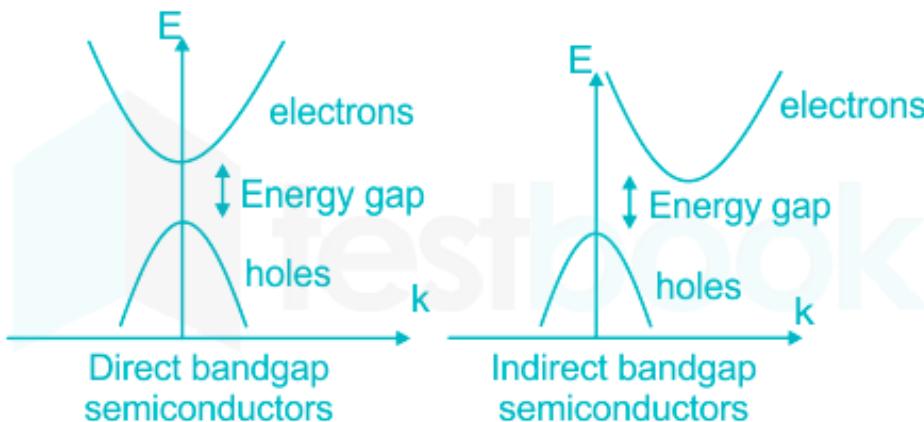
Gallium arsenide offers significant advantages over silicon, such as higher electron mobility and better performance in optoelectronic applications due to its direct bandgap. Silicon is an indirect band gap semiconductor with a band gap of 1.2 eV.

Drawbacks for GaAs: Higher manufacturing costs, more brittle compared to silicon.

Toxicity studies in experimental animal systems have shown gallium nitrate and gallium arsenide to produce toxicity to the lungs, immune system, kidneys, and hematopoietic systems. The International Agency for Research on Cancer (IARC) has classified gallium arsenide as a human carcinogen.

Direct Band Gap (DBG) Semiconductors:

The semiconductor in which the top of the valence band and the bottom of the conduction band occur at the same value of momentum.



<https://testbook.com/objective-questions/mcq-on-direct-and-indirect-band-gap-semiconductors--5eeaa0c39140f30f369dfa4>

Since Silicon is an Indirect Band Gap semiconductor so electron cannot fall directly to the valence band but must undergo a momentum change as well as a change in energy. So, energy is released as heat along with light.

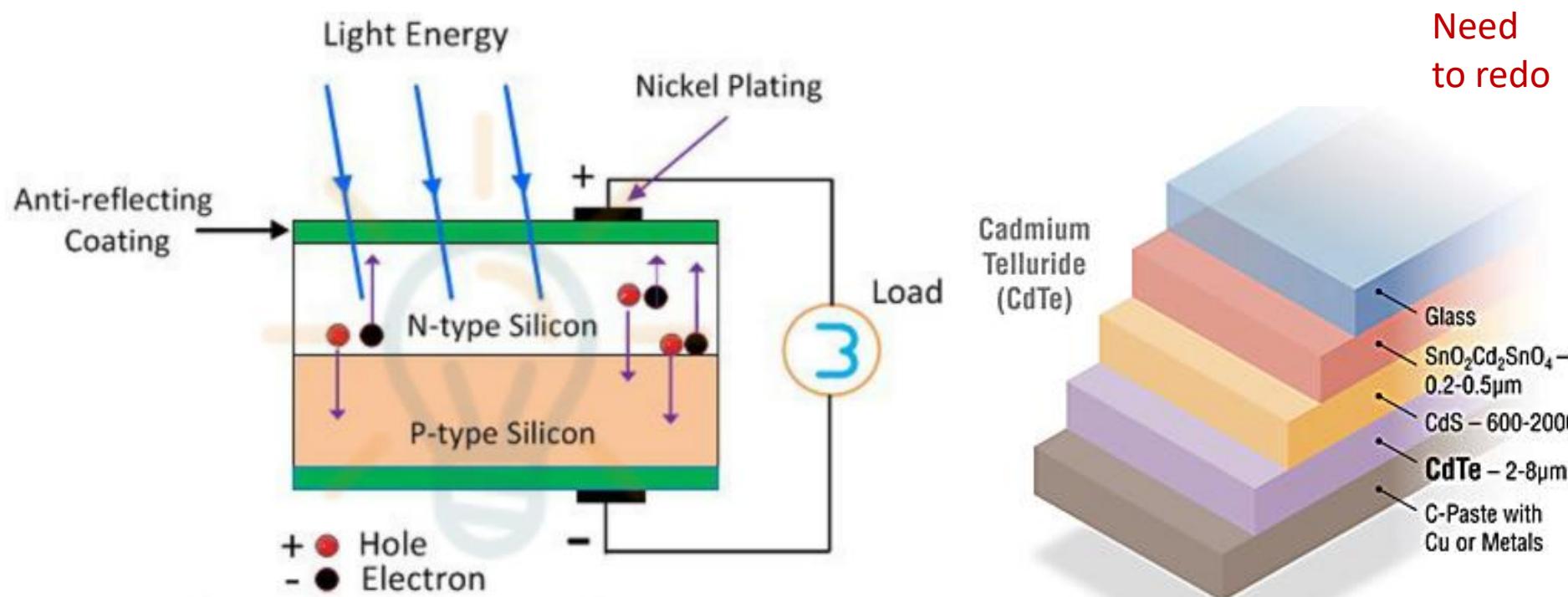
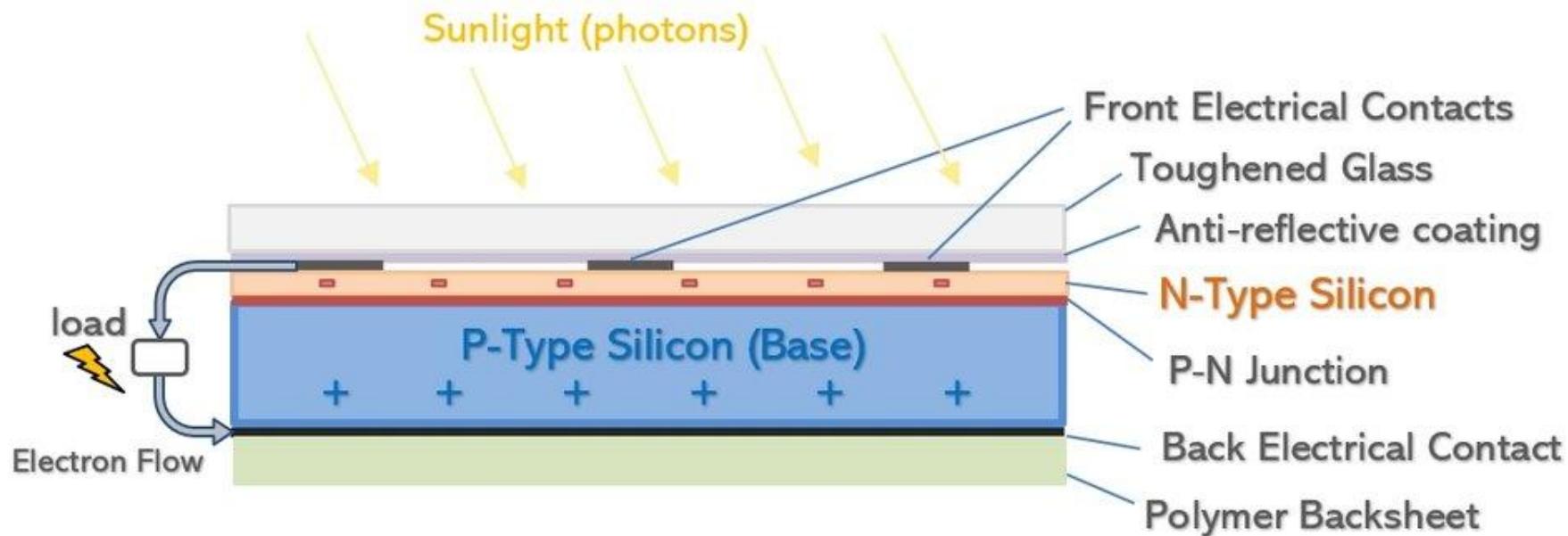
Type of Solar Panel	Pros	Cons
Monocrystalline	<ul style="list-style-type: none"> Highest efficiency, which means more kilowatt-hours per square foot covered. Longer lifespan (25+ years) 	<ul style="list-style-type: none"> Most expensive type of solar panel
Polycrystalline	<ul style="list-style-type: none"> Balanced cost and efficiency: intermediate between monocrystalline and thin-film solar panels (best suited for installations where space is not a constraint). Long lifespan (25+ years) 	<ul style="list-style-type: none"> Lower efficiency than mono panels Higher temperatures affect productivity and durability
Amorphous	<ul style="list-style-type: none"> High temperatures only have a small impact on their productivity. Lightweight Low cost Flexible and adhesive panels are available 	<ul style="list-style-type: none"> Low efficiency, which means unfit for the average home Shorter lifespan than mono and poly panels

<https://www.ecowatch.com/amorphous-solar-panels.html>

Amorphous silicon (a-Si) is the non-crystalline form of silicon used for solar cells. Used as semiconductor material for a-Si solar cells, or thin-film silicon solar cells, it is deposited in thin films onto a variety of flexible substrates, such as glass, metal and plastic.

Amorphous silicon cells generally feature low efficiency, but are one of the most environmentally friendly photovoltaic technologies, since they do not use any toxic heavy metals such as cadmium or lead.

Property	Amorphous Si (a-Si)	Crystalline Si (c-Si)
Process temperature	Low (200–400 °C)	High (>1000 °C)
Fabrication ease	Easy, large-area deposition	Complex, wafer-based
Processibility	High	Low
Electrical performance	Low	High



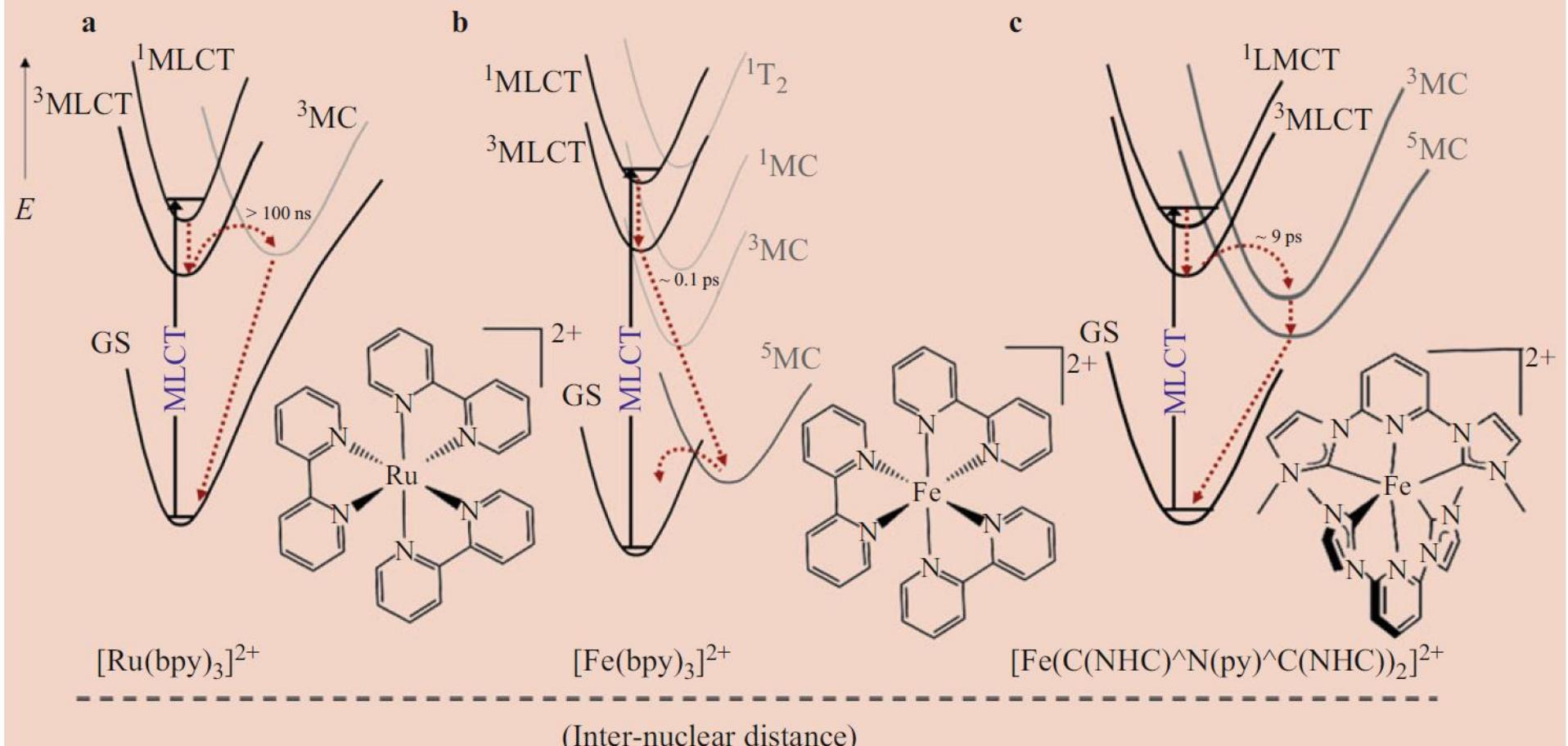


Fig. 20.3 Comparison between the potential energy diagram for the excited states of selected d^6 complexes (a) $[\text{Ru}(\text{bipy})_3]^{2+}$ [30], (b) $[\text{Fe}(\text{bipy})_3]^{2+}$ [31], and (c) $[\text{Fe}(\text{C}(\text{NHC})^{\wedge}\text{N}(\text{py})^{\wedge}\text{C}(\text{NHC}))_2]^{2+}$ [32]

Feature	$[\text{Fe}(\text{bpy})_3]^{2+}$	$[\text{Ru}(\text{bpy})_3]^{2+}$
Metal	$\text{Fe}(\text{II}), \text{3d}^6$	$\text{Ru}(\text{II}), \text{4d}^6$
Ligand field strength	Moderate	Strong
MC state energy	Low-lying	High-lying
MLCT lifetime	<100 fs	$\sim 1 \mu\text{s}$
Emission	Quenched (none)	Strong MLCT phosphorescence

Third Generation Solar Cells DSSC

Need
to redo

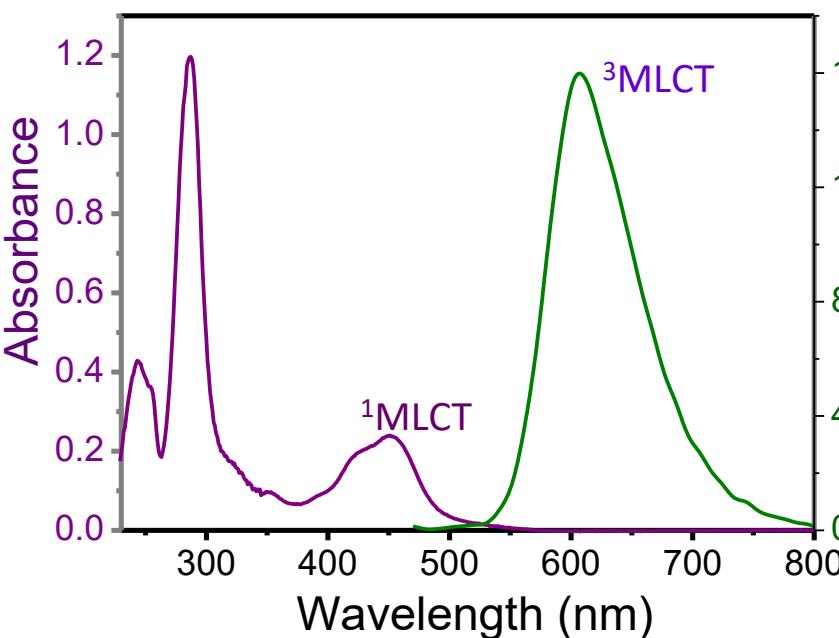
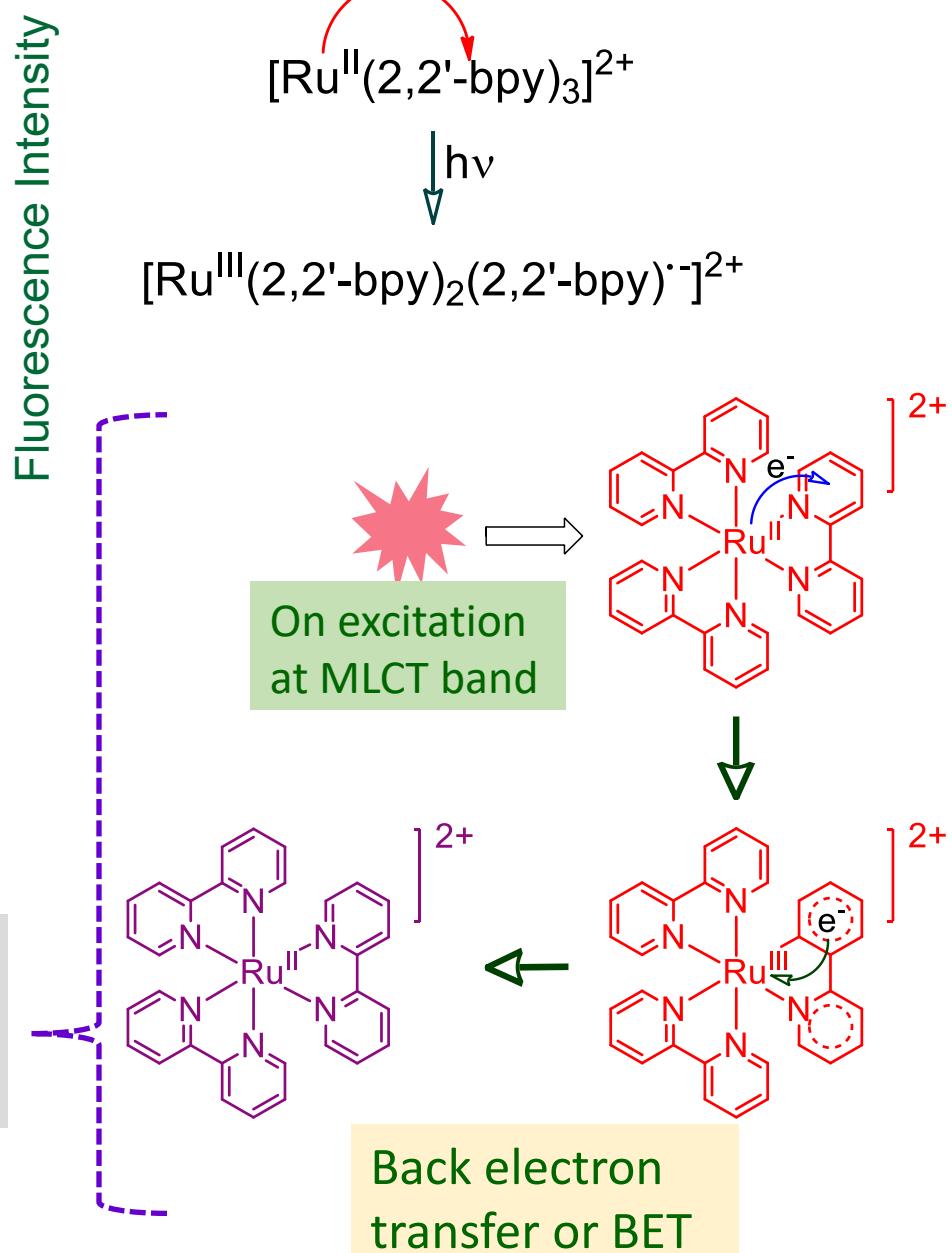


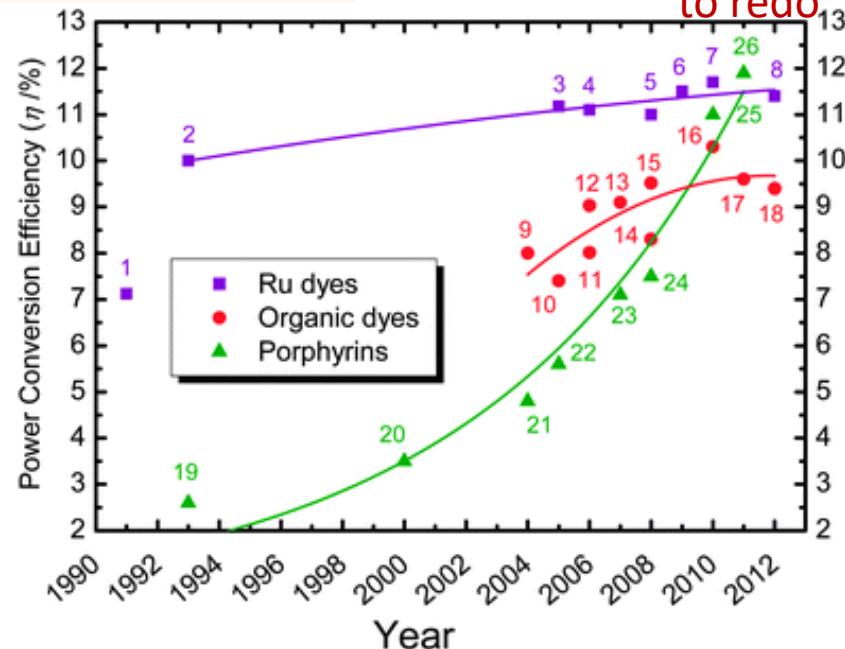
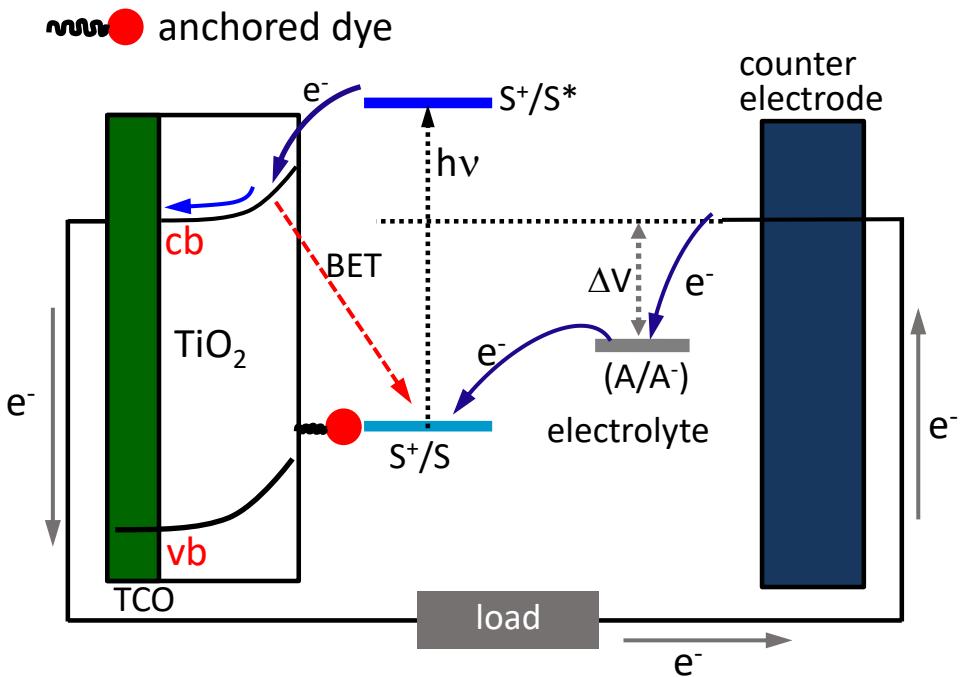
Photo-induced e^-
transfer Processes

Fast BET process is generally not
desired for the design of an efficient
Dye Sensitized Solar Cell (DSSC).



The Dye Sensitized Solar Cell

Need
to redo



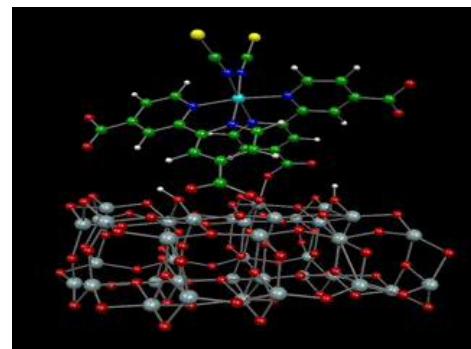
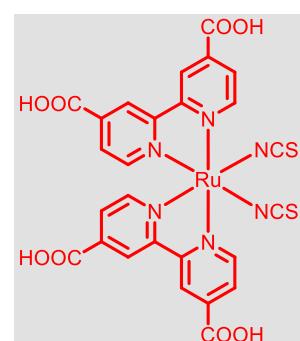
Diau et. al. Chem. Soc. Rev. , 2013, 42, 291-304

Carboxylate binding has undoubtedly been the most promising so far.....

Limitation:Sensitizers bound to metal oxide surfaces through this linkage exhibit high stability in most anhydrous organic solvents and in acidic aqueous solution only; in neutral and basic aqueous solutions the sensitizers are rapidly desorbed from the surface.

This is due to the related protolytic equilibrium; the ground state pK_a of carboxylates is too low to ensure strong binding.

Kalyanasundaram, Coord. Chem. Rev. 1998, 77, 347

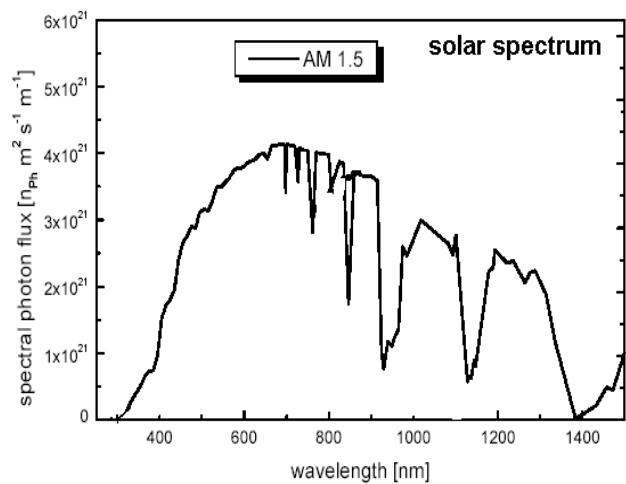
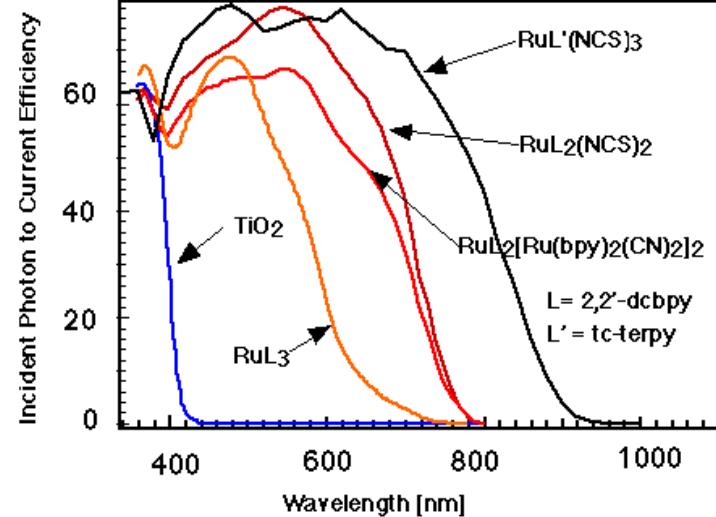
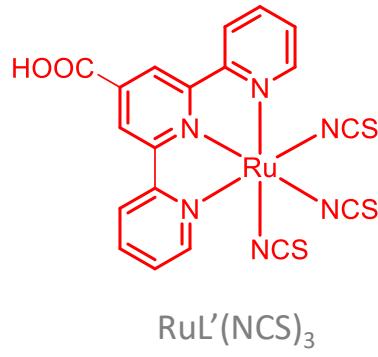
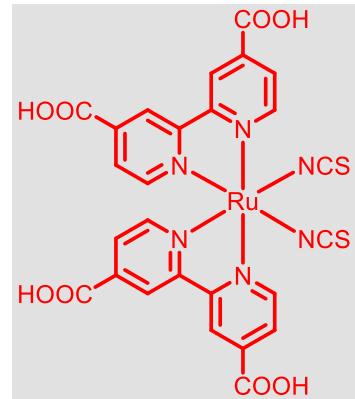


M. Graetzel, Nature, 2001, 414, 338.;
Inorg. Chem. 2005, 44, 6841

BET happens in μ s

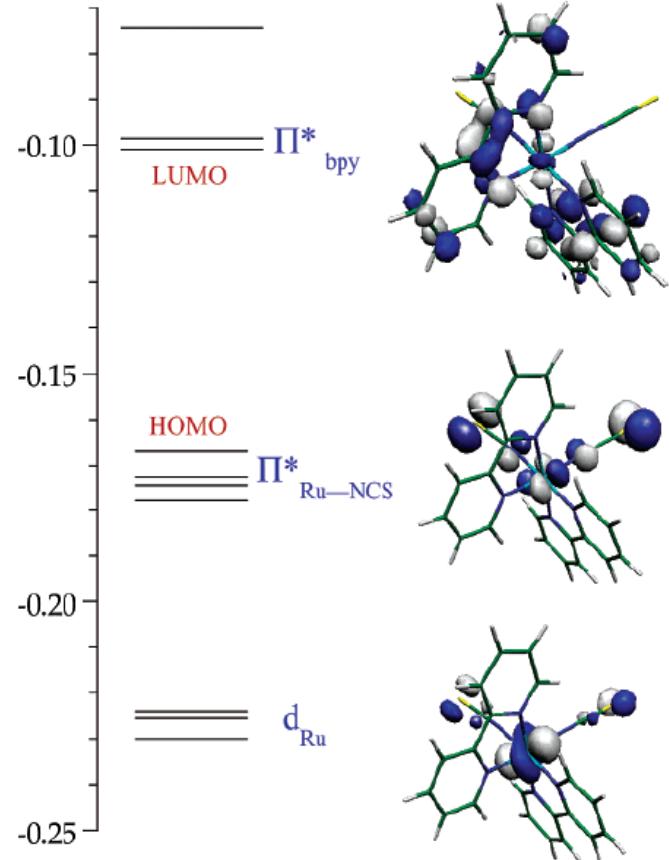
Dyes used in Grätzel Solar Cell

Efficiency of about 12% has been reported

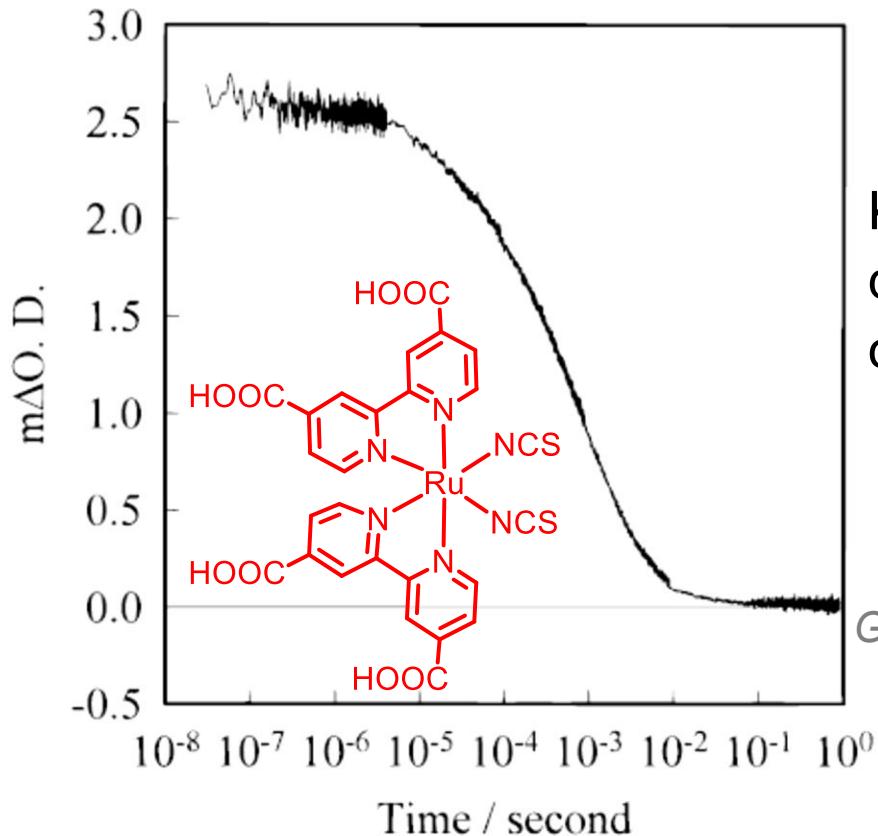


E (hartrees)

Why -SCN ?



Grätzel dye
Photophysics



Kinetics of charge recombination of the dye-coated TiO_2 film, monitored by decay of the cation absorption band at 820 nm.

Grätzel et. al; *Nature* 1991, 353, 737

J. Phys. Chem. 1996, 100, 20056

Account of Chem. Res. 2009, 42, 1788.

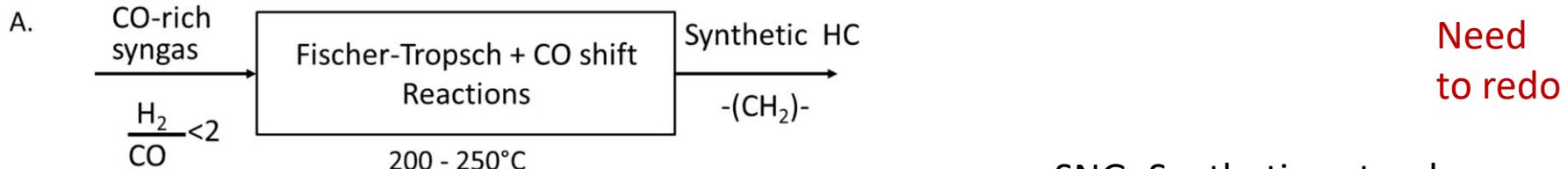
Disadvantages with carboxylate as anchoring group:

The ground state pK_a of the carboxylates is too low to ensure strong and in presence of water, slow desorption of the photosensitizers can occur which can limit the long-term stability of the cell.

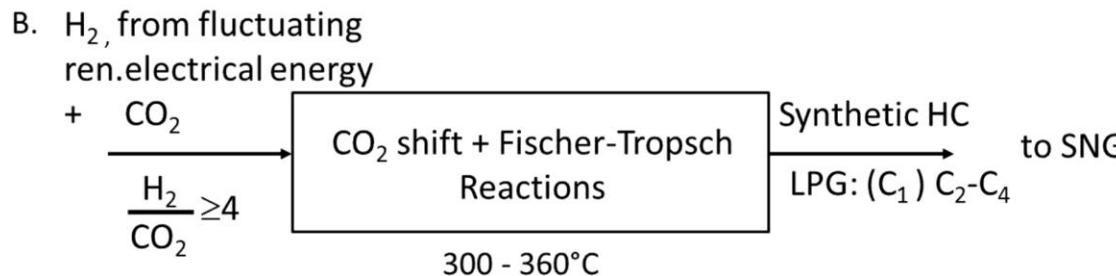
Phosphonate has also been investigated as anchoring groups; phosphonates ($\text{pK}_\text{a} \sim 6.5$) provide stronger binding than carboxylates ($\text{pK}_\text{a} \sim 4$). However, these anchoring functionalities have intrinsic problems with slow dissociation of the dye.

Table 1. List of standalone (S) and hybridized (H) FPV co-benefits reviewed in this paper (S = standalone FPV, H = hybridized FPV) [33–42,49].

Social	Economic	Energy	Water	Food or Land
Reduces land use (S, H)	Increases ease of installation (S, H)	Increases panel efficiency (S)	Reduces evaporation (S, H)	Reduces land use (S, H)
Repurposes otherwise unusable land (S, H)	Reduces site preparation (S, H)	Increases panel packing density (S, H)	Reduces algae growth and improves water quality (S, H)	Repurposes otherwise unusable land (S, H)
Preserves valuable land and water for other uses (S, H)	Modular (S, H)	Reduces shading (S, H)	Reduces water temperature (S, H)	Increases energy sources near demand or population centers (S, H)
Avoids or reduces conflicts over land and water use (S, H)	Uses existing electrical transmission infrastructure (S, H)	Increases panel efficiency (H)	Provides power during drought (H)	
Reduces or avoids power-generation related air-pollution (S, H)	Reduces curtailment (H)	Improves power quality (H)	Reduces wave formation (S, H)	
Reduces displacement of local communities for energy development (S, H)	Improves power quality (H)			
Improves power sector resilience (S, H)	Extends system life (S, H)			

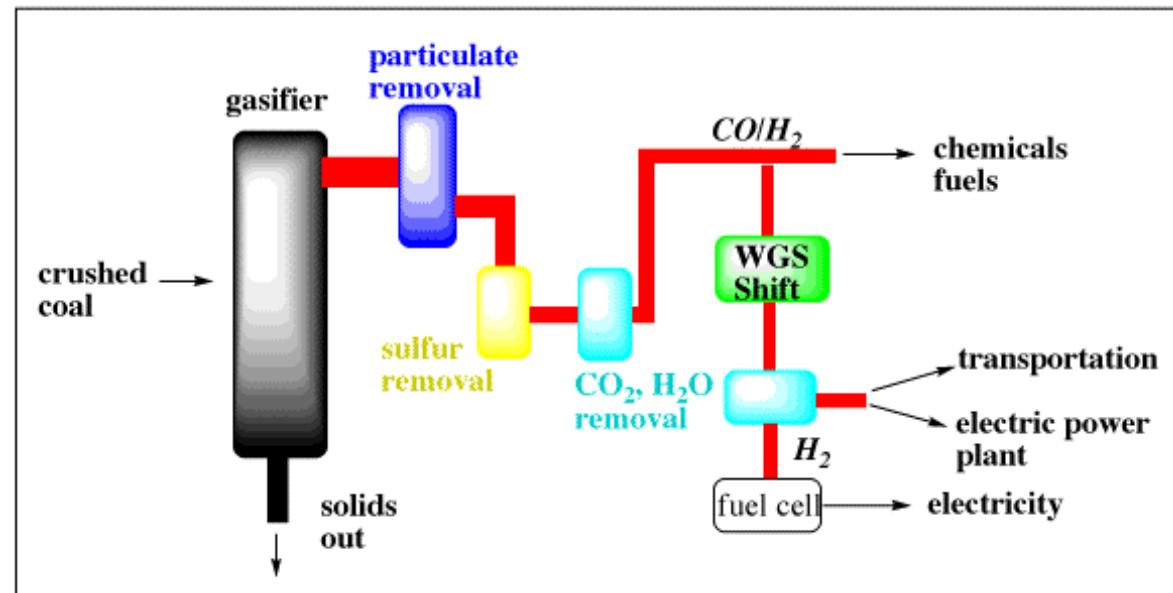


SNG: Synthetic natural gas



Water gas is a kind of fuel gas, a mixture of CO and H₂. It is produced by "alternately hot blowing a fuel layer [coke] with air and gasifying it with steam.

In the gasifier, crushed coal is combined with steam at high pressure and temperature. The quantity of oxygen is limited to prevent the complete combustion of coal. Instead, the carbon reacts with the steam to form a mixture of CO, H₂, and other gases.



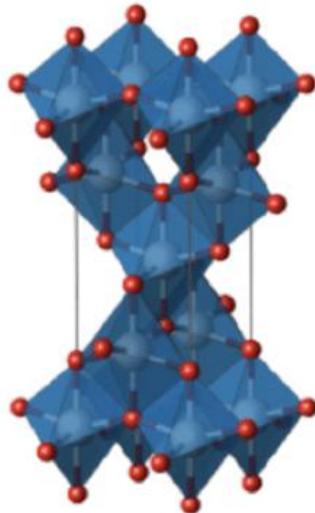
- Coal as fuel contributes to ~ 50% of the electricity generation in India. Coal is more abundant than oil and coal reserves are far more abundant than oil reserves in this world.
- Coal burning enhances the CO₂ footprint. Burning coal results in NOx and SOx, heavy metals (such as Hg), and radioactive metals, which need to be cleaned. Apart from these coal burning adds to a significant amount of ash.
- This is why we need clean coal technology.

Mercury in coal is released to flue gases in the form of Hg⁰ during combustion in a thermal power plant. Decreasing temperature from over 800°C to below 300°C in flue gases leaving boilers or furnaces promotes oxidation of Hg⁰ to gaseous Hg²⁺, with a portion of Hg²⁺ adsorbed onto fly ash to form particulate-bound mercury (Hg_p)

The overall trend is not on track with the Net Zero Emissions by 2050 Scenario, which calls for immediate reductions and a global decline in unabated coal-fired generation of around 55% by 2030 compared to 2022 levels, and a complete phase-out by 2040. About 70% of world steel production depends on coal feedstock. Coal is the world's most abundant and widely distributed fossil fuel source.

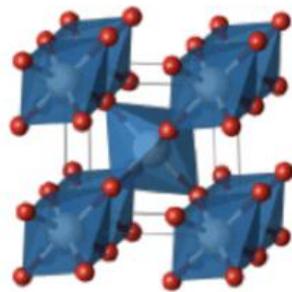
Titanium dioxide, the only naturally occurring oxide of titanium at atmospheric pressure, exhibits three polymorphs: **rutile**, **anatase**, and **brookite**. While rutile is the stable phase, both anatase and brookite are metastable; the latter is difficult to synthesize.

Anatase



Octahedra form
(001) planes;
Band gap: 3.2 eV

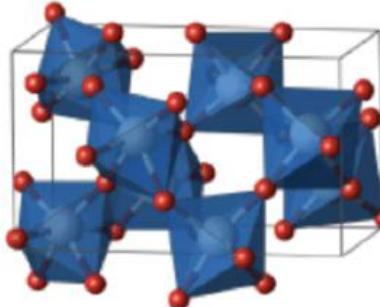
Rutile



Eight share corners and
only two share edges
running along the [110]-
type direction.

Thermodynamically most
stable phase.
Band gap: 3.0 eV

Brookite



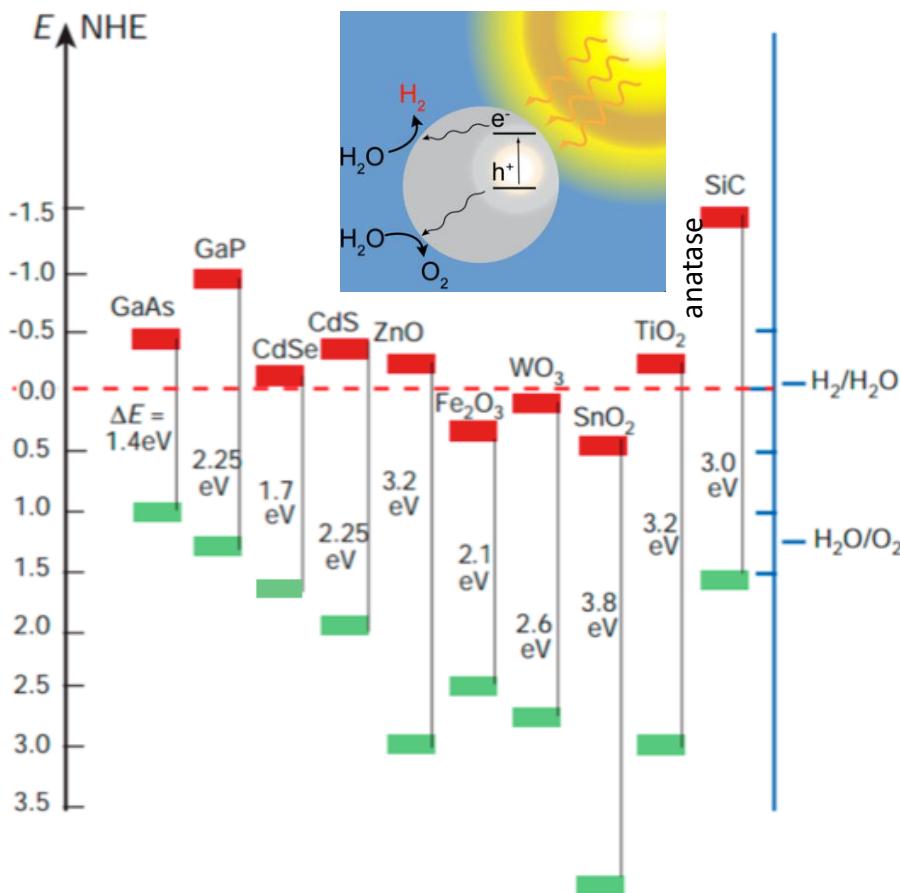
Orthorhombic unit
cell, each octahedron
shares three edges.
Band gap: 3.0 – 3.4 eV

The small red spheres represent the oxygen atoms, the big grey ones are the titanium atoms, while the blue polyhedral shapes show the orientation in space of the TiO_6 octahedra.

Degussa P25 nanopowder, a mixture of 75% anatase and 25% rutile, is often employed as a reference photocatalyst in photocatalytic studies and industrial applications. P25 generally displays enhanced photocatalytic performance over pure rutile or anatase nanocrystals

Generally, anatase is more active than rutile, but no consensus exists to explain this difference.

Propositions: For anatase the activity increases for films up to 5 nm thick, while rutile films reach their maximum activity for 2.5 nm films. Presumably, the charge carriers excited deeper in the bulk contribute to surface reactions in anatase than in rutile. A better bulk charge diffusion perhaps favours the improved photocatalytic activity of anatase.



Energy band positions (CB in red, VB in green) for some selected semiconductors in contact with an aqueous electrolyte at pH 1 with respect to the standard hydrogen electrode (NHE) and the vacuum level as a reference. For TiO_2 only the anatase level alignments are shown.

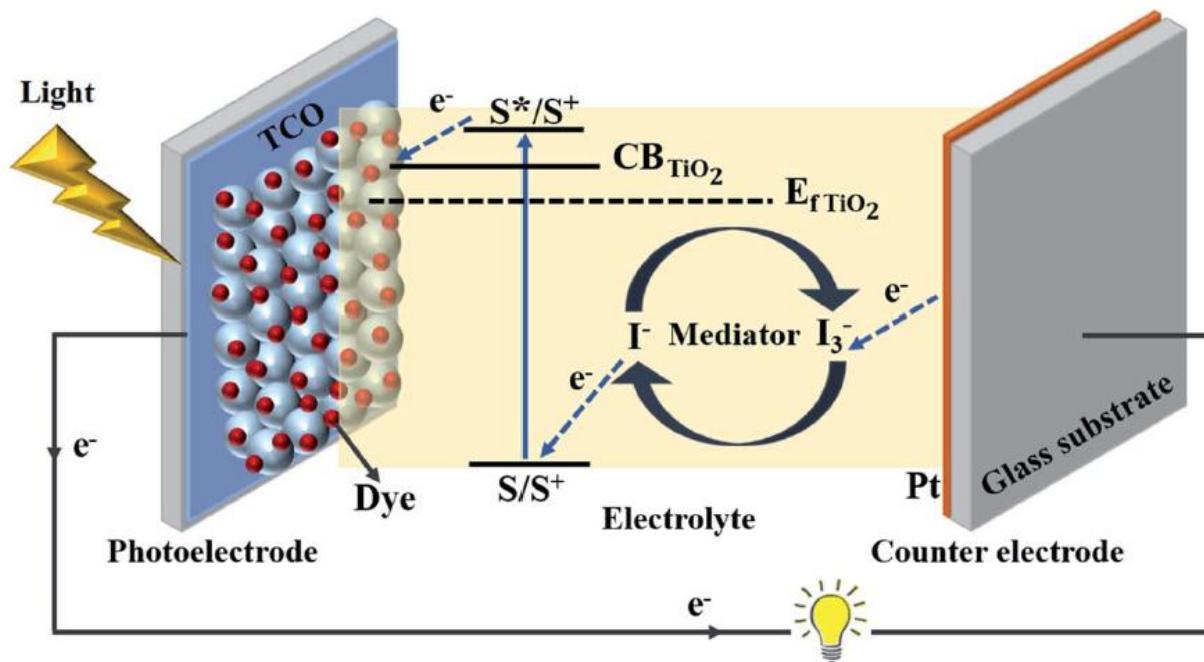


Fig. 2 Schematic illustration representing device structure and working principle of a dye-sensitized solar cell. CB = conduction band, $E_f \text{TiO}_2$ = fermi level of TiO_2 , S = ground state of dye sensitizer molecule, S^* = excited state of dye sensitizer molecule, S^0 = oxidized dye, S^+ = charge separation, I^- = iodide ion and I_3^- = triiodide ion.

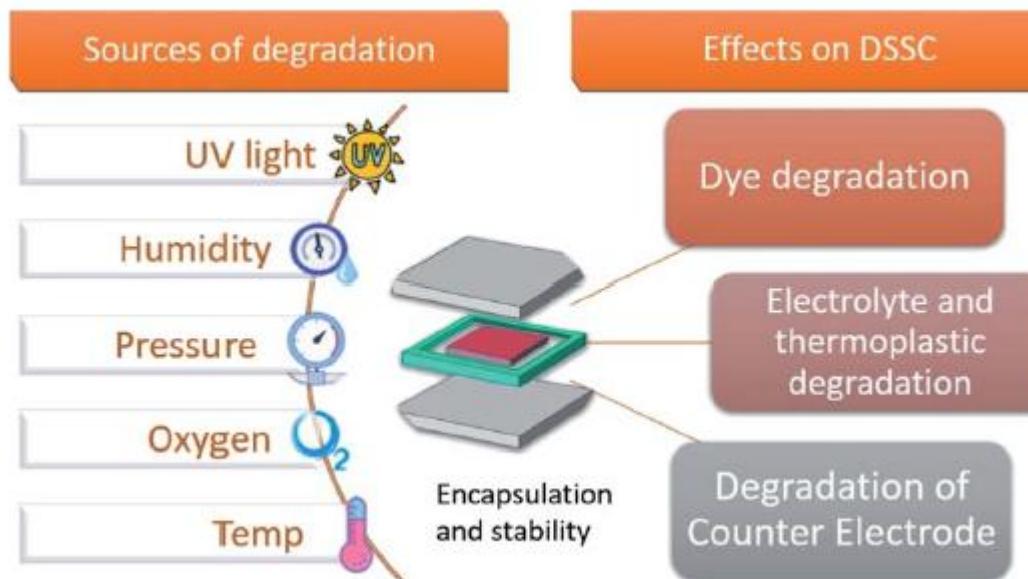
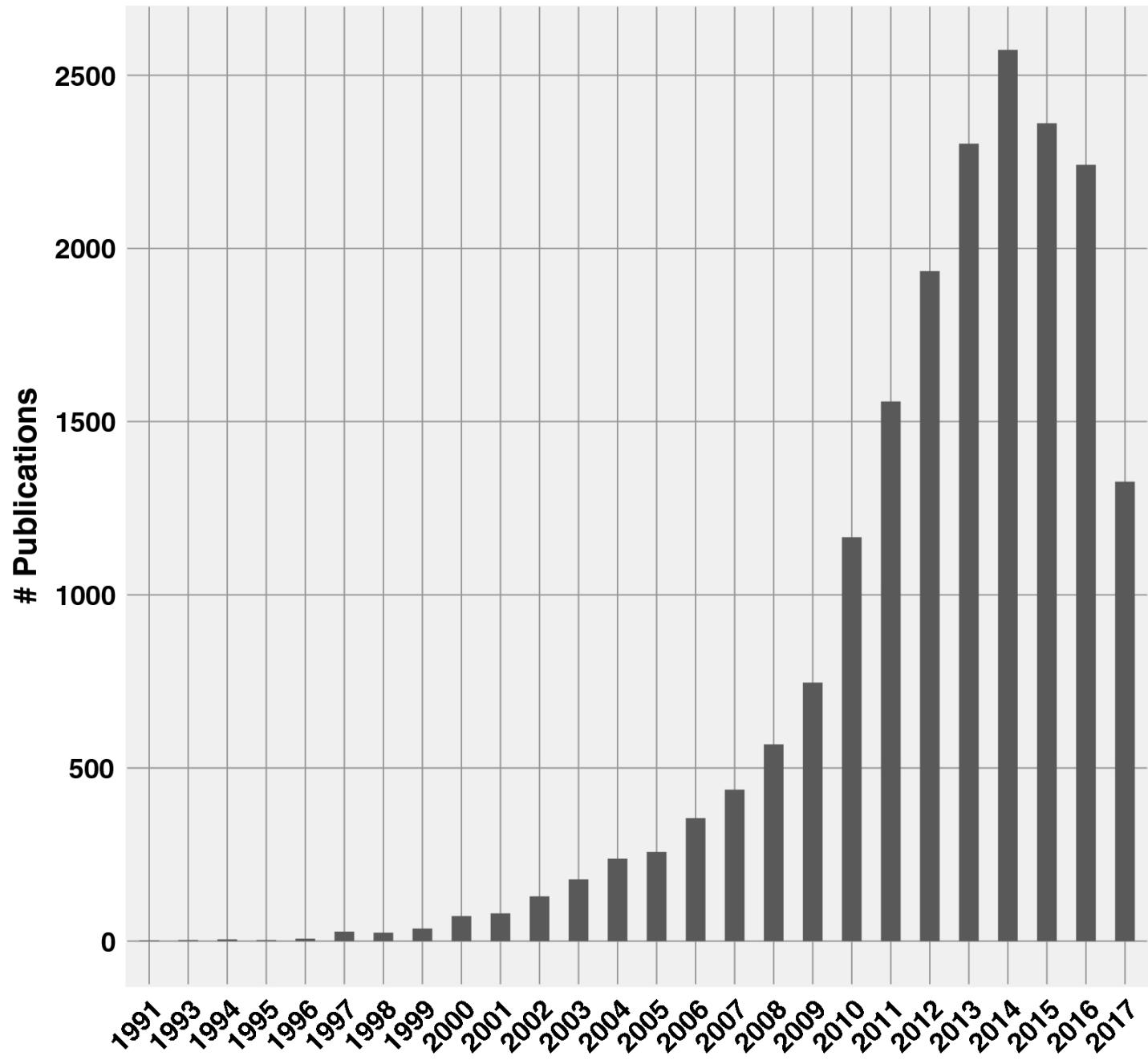


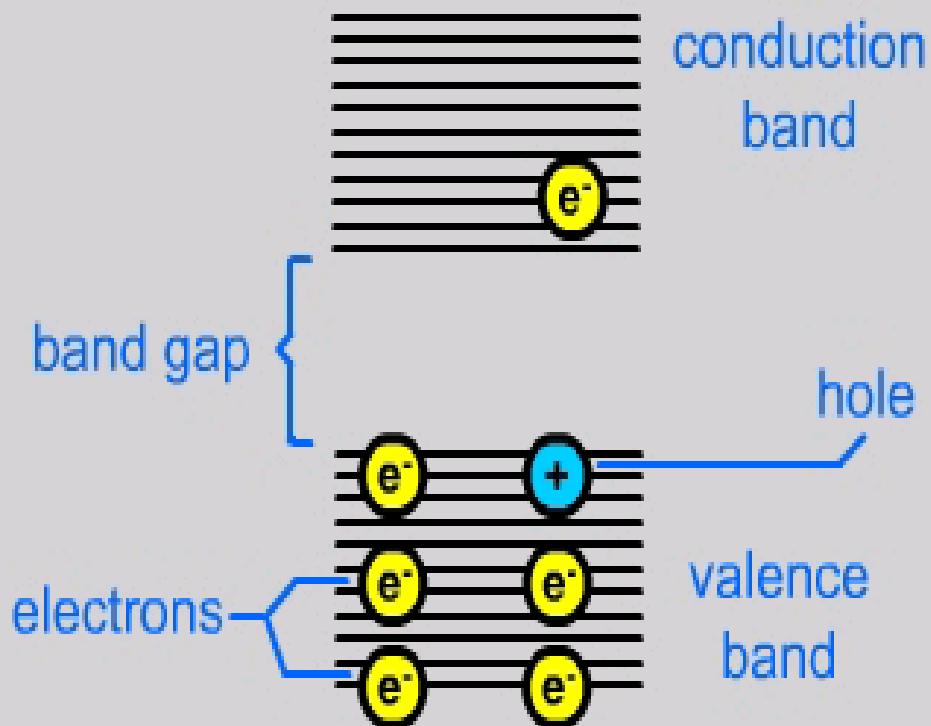
Illustration of the factors that affect DSSC devices and their possible consequences which hinder the photovoltaic performance



Quantum Dot Solar Cell

- The average distance between an electron and a hole in an exciton is called the **Excited Bohr Radius**.
- When the size of the semiconductor falls below the Bohr Radius, the semiconductor is called a quantum dot.

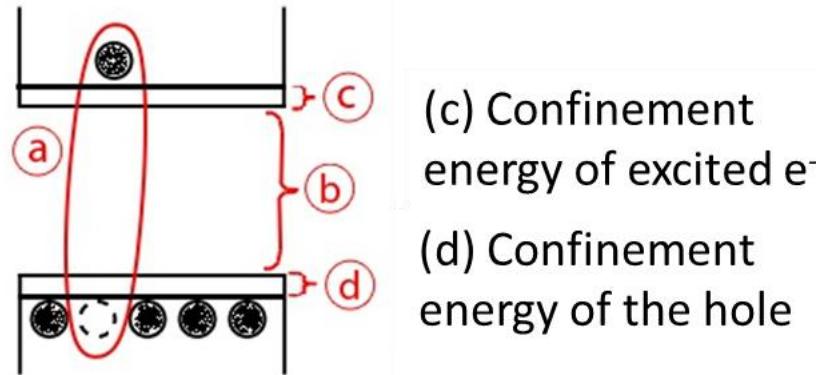
SEMICONDUCTOR energy levels



Quantum dot solar cells have the potential to produce high efficiencies with a relatively cheap cost to construct them. Furthermore, quantum dots have the capability of multiple electrons being excited from one photon of light (in comparison to organic dyes which generally only have one electron excited per single photon)

- (a) exciton
- (b) bandgap

Quantum confinement effect

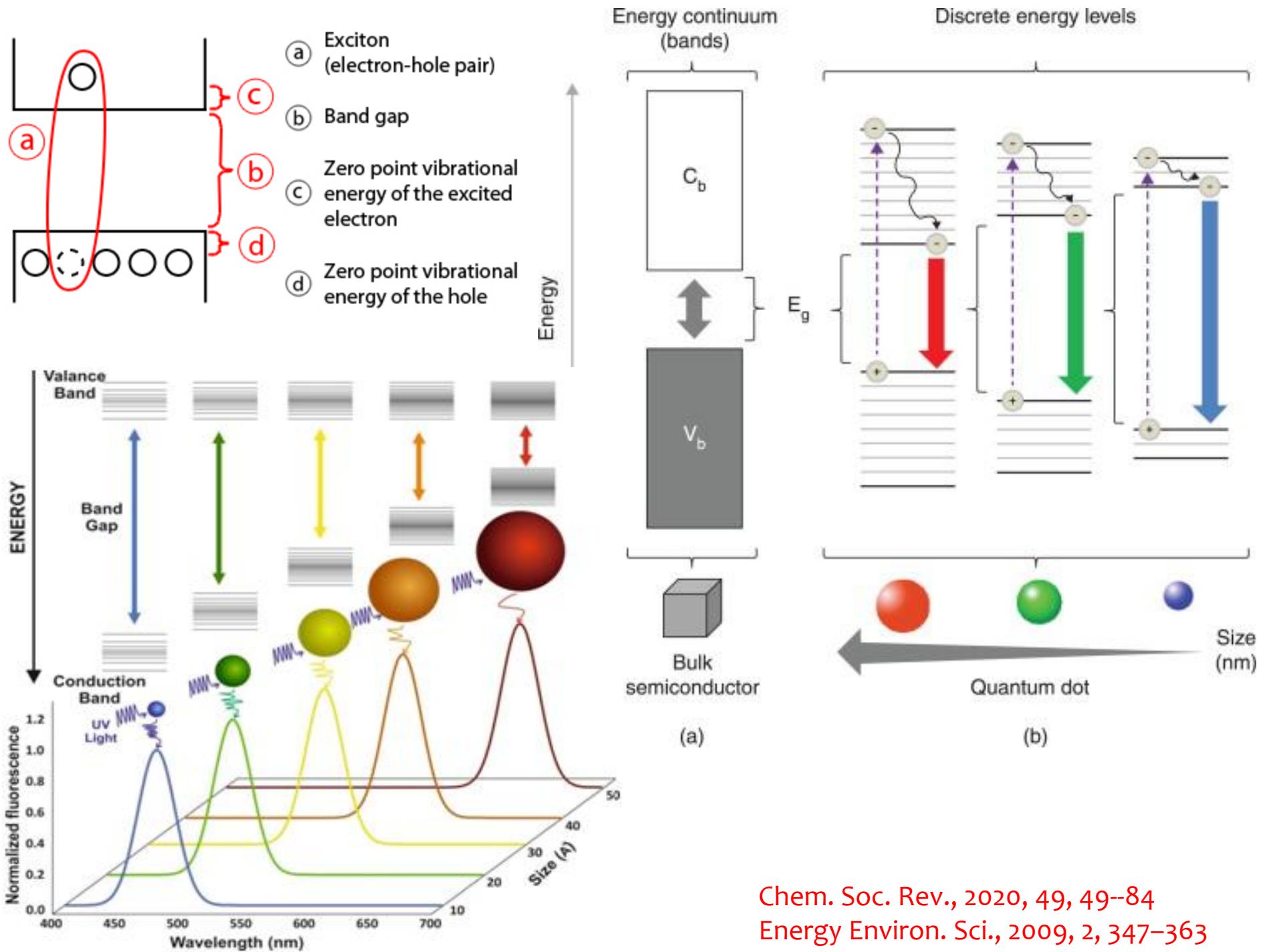


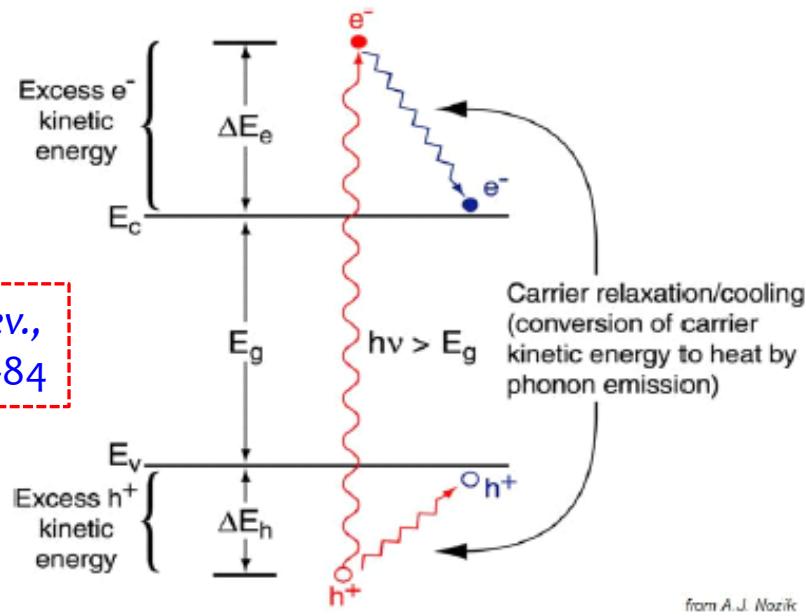
- (c) Confinement energy of excited e⁻
- (d) Confinement energy of the hole

Generally, when the size of the quantum dot is equal to or smaller than the exciton Bohr radius of the corresponding bulk material, the movement of the carrier electron-hole pair is in a strongly restricted state. As the particle size becomes smaller, the energy gap increases and the energy in the semiconductor material is quantified. The energy after quantification of the semiconductor material is:

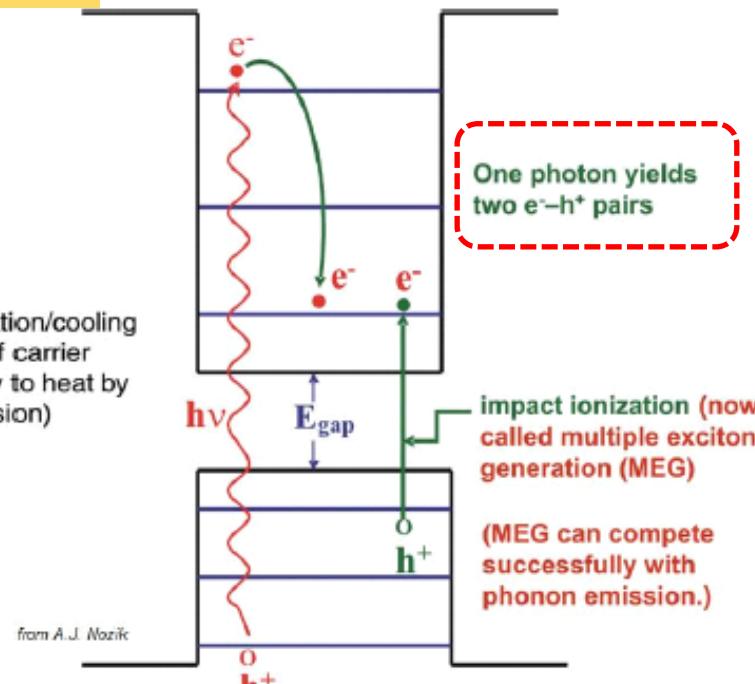
$$\Delta E_g = E(R) + [h^2 / 8R^2 (1/m_e + 1/m_h)] \quad [E(R) \text{ is the lowest excitation energy}]$$

In the formula, ΔE_g is the bulk band gap, m_e and m_h are the mass of electrons and holes, respectively, R is the radius of the particle, and $E(R)$ is the lowest excitation energy.





(a) Bulk Semiconductor



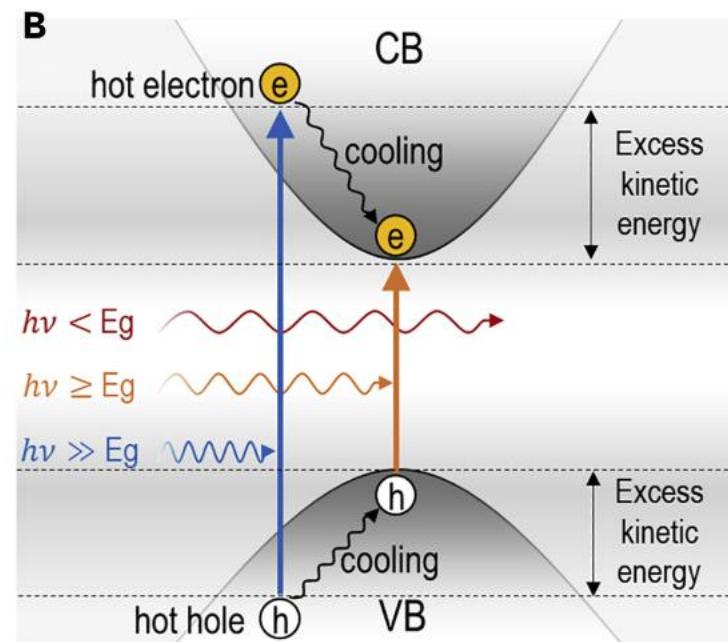
(b) Quantum Dot

From A.J. Nozik

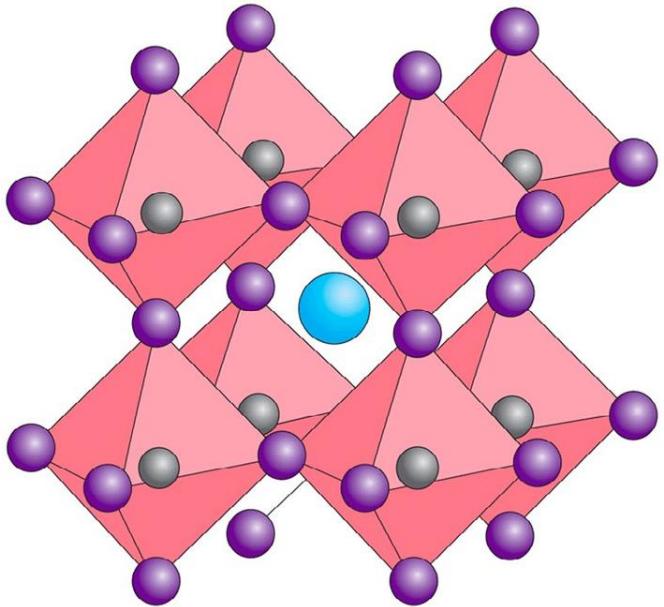
In **Bulk Semiconductor** hot electrons and holes release the excess energy to the band gap energy via successive emission of phonons and cool to the band edge quickly within femtosecond and the excess energy is lost in the form of heat energy. It is difficult to extract the electrons from their higher energy state.

For **QDs** the cooling process becomes slower and electrons with excess energy more than the band gap energy can create another electron-hole pair known as multiple exciton generation, which could enable QDSCs to break the Shockley–Queisser efficiency limit of 32.9 % for a single junction (single absorber) solar cells.

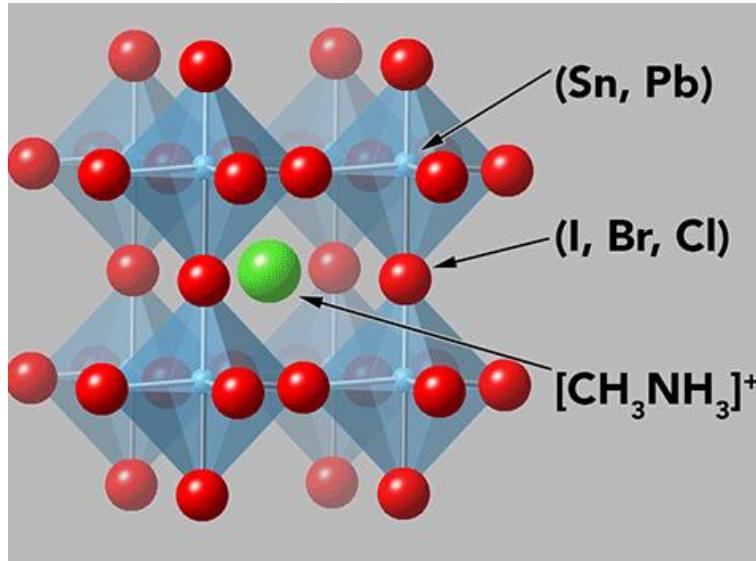
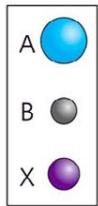
The Shockley–Queisser (SQ) limit describes the theoretical sunlight-to-electricity conversion efficiency of a single-junction solar cell. The SQ limit (33.7% under AM1.5g illumination (109,870 lux). SQ limit refers to the maximum theoretical efficiency of a single-junction solar cell and is calculated by examining the amount of electrical energy extracted per incident photon. Using an AM 1.5 solar spectrum, a solar cell with an ideal band gap light absorber (band gap, $E_g = 1.4$ eV) could have an upper limit on PCE of 33.7%,⁶ i.e., a maximum electrical power generation of 337 W m⁻². A major loss factor is related to the energy mismatch between the broad wavelength distribution of sunlight and the mono-band gap of the light absorber in the cell.



The terms "perovskite" and "perovskite structure" is a type of mineral that was **first found in the Ural Mountains and named after Lev Perovski** (the founder of the Russian Geographical Society). True perovskite (the mineral) is composed of calcium, titanium and oxygen in the form CaTiO_3 . Meanwhile, a perovskite structure is anything that has the generic form ABX_3 and the same crystallographic structure as CaTiO_3 .



Nat. Photonics.
2014;8:506–514



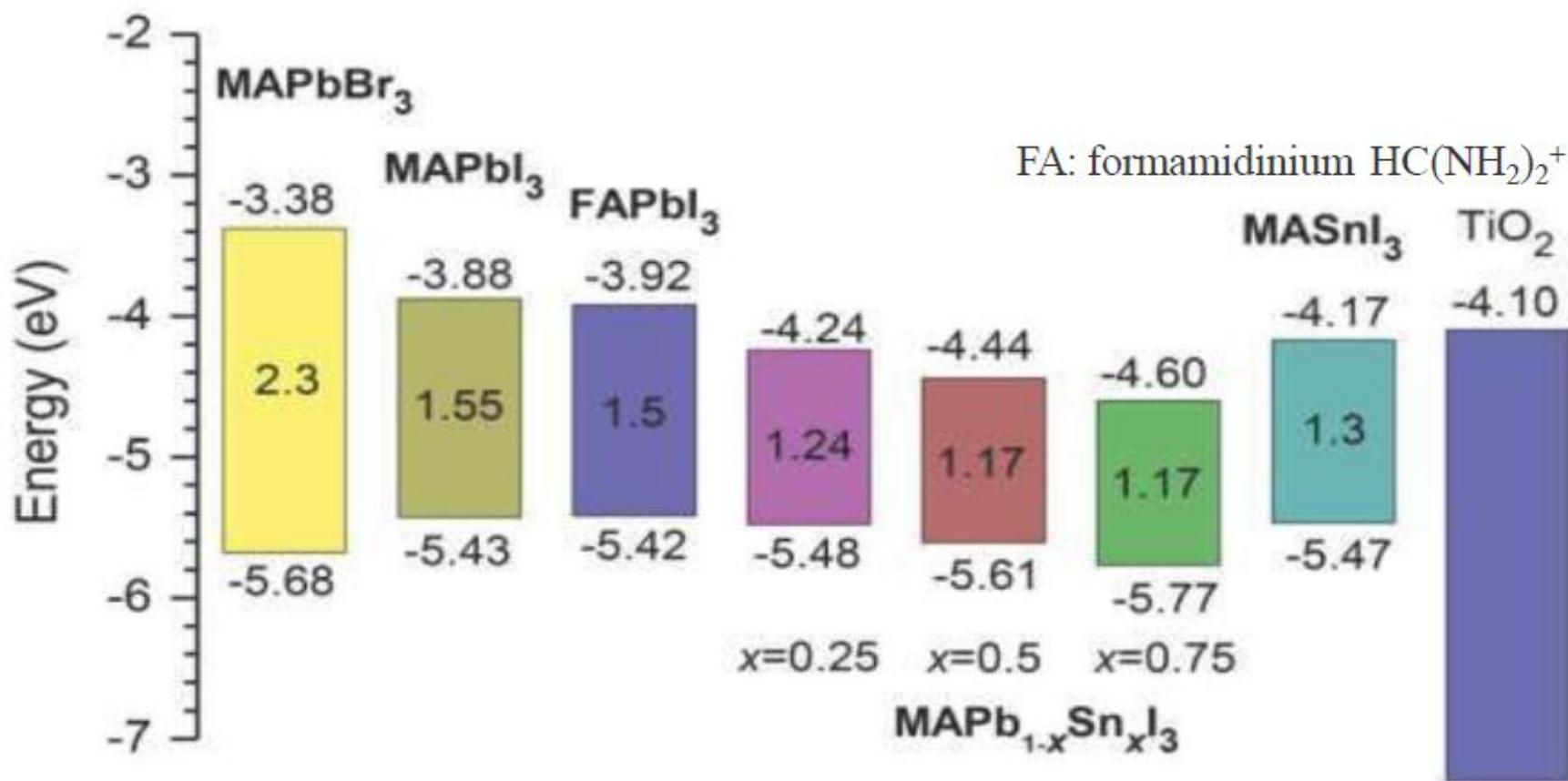
Science, Vol. 2012, 338, 643–647

Perovskites were first successfully used in solid-state solar cells in 2012, and since then most cells have used the following combination of materials in the usual perovskite form ABX_3 :

A = An organic cation - CH_3NH_3^+ or $\text{NH}_2\text{CHNH}_2^+$; **B** = A big inorganic cation - usually Pb^{2+} & **X** = A halogen anion – usually Cl^- or I^-

BAND GAP TUNING is Important for having wider and longer wavelength absorption without sacrificing the absorption coefficient.

Changing in any of A, M and X in AMX_3 or by varying the ratio of Pb to Sn helps in tuning band gap



Mesoporous TiO₂ layer is usually used to collect the electrons.

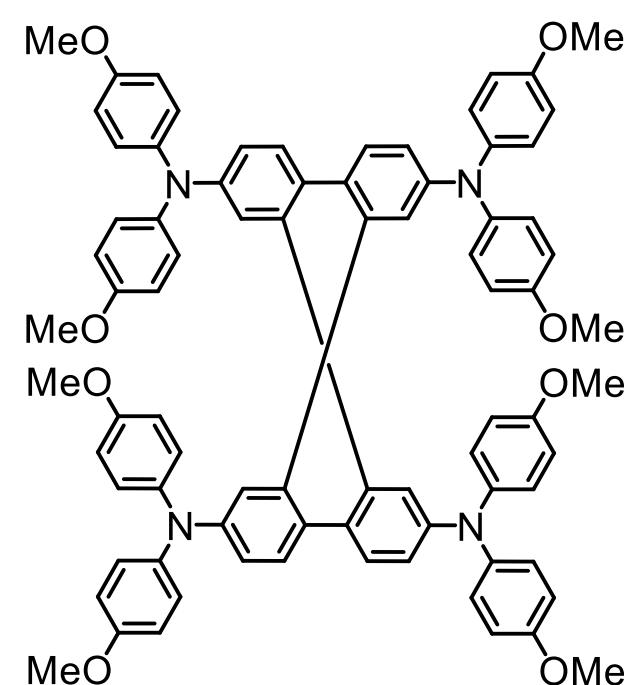
Organic Hole transporting material (HTM) collects the holes.

ORGANIC-INORGANIC HYBRID PEROVSKITES

- Hybrid Organic Inorganic Semiconductor
- Inorganic - Lead (Strong light absorption, Provide high efficiencies, even above 20 % as per NREL)
- Organic- Methyl Ammonium (Soluble in Polar Solvents, Provides low temperature processing - low cost and energy saving)
- First three-dimensional organic–inorganic hybrid perovskite:
Replacing Cs^+ in CsPbX_3 ($X = \text{Cl}, \text{Br}$ or I) with MA (CH_3NH_3)⁺ in 1978.
- $\text{CH}_3\text{NH}_3\text{PbI}_3$ is most common used materials for making high efficiency perovskite solar cells.

The majority of efficient perovskites are based on Group IV (specifically, lead) metal halides. Lead-based perovskite solar cells are particularly good because of a range of factors, including strong absorption in the visible regime, long charge-carrier diffusion lengths, a tunable band gap, and easy manufacture (due to the high defect tolerance and the ability to process at low temperatures).

The highest efficiency potential (approx. 35%) is computationally predicted for an optimum perovskite band gap of approximately 1.7 eV. However, many perovskite compositions with such a band gap are unstable as they feature a mix of iodide and bromide on the halide X-position with a **high bromide content, leading to halide segregation under illumination — so-called photo-instability**. To avoid photo-instability, most literature on perovskite silicon tandem devices implement a perovskite composition featuring a reduced bromide content and, thus, a smaller band gap.



Due to the lack of planarity, organic modifications not to affect the ionization potential appreciably.

Typical properties:

HOMO = -5.15 eV

$$E(\text{eV}) = 1240 \lambda \text{ (expressed in nm)}$$

LUMO = -2.10 eV

$E_{\text{ox}}(\text{DCM}) = 0.65 \text{ V vs. NHE}$

Hole mobility = $1.9 \times 10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$

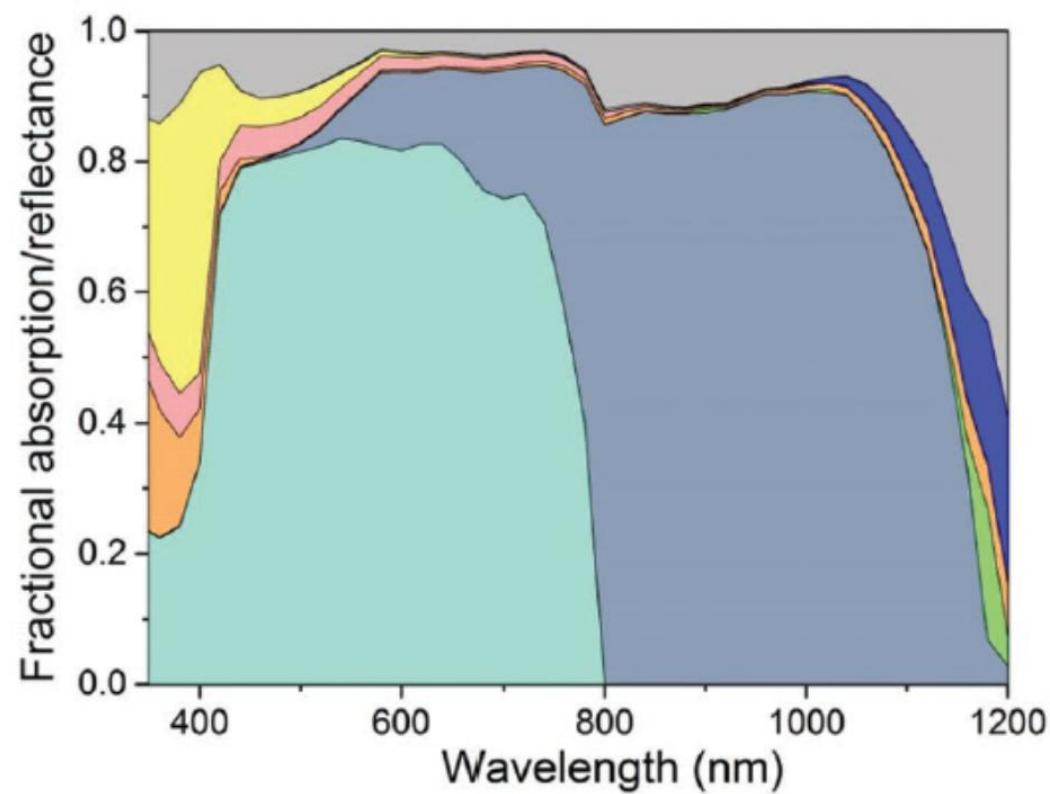
$\lambda_{\text{abs}} = 387 \text{ nm}$

Energy & Environmental Science,
2016, DOI: [10.1039/C6EE00056H](https://doi.org/10.1039/C6EE00056H)

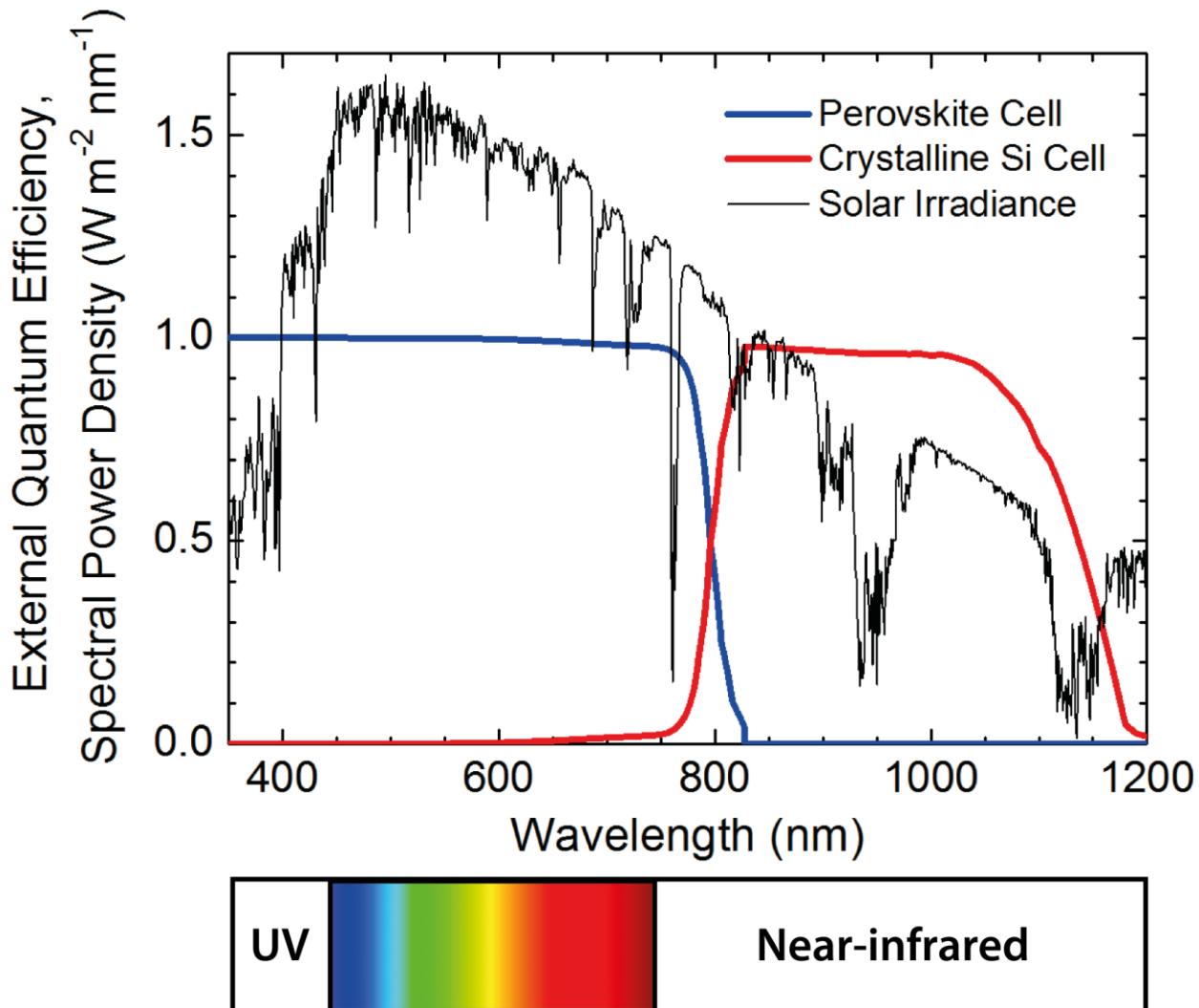
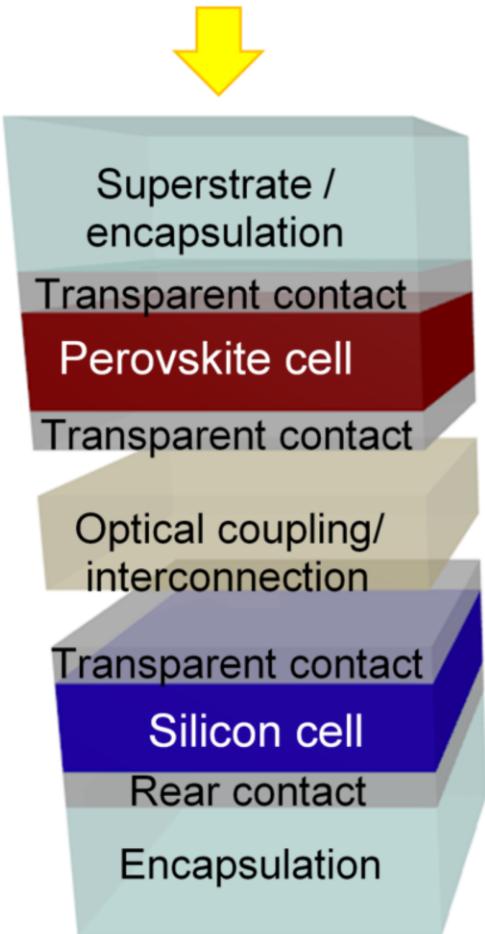
A prominent solid-state HTM is **2,2',7,7'-tetrakis(N,N-di-p-methoxyphenyl-amine)9,9'-spirobifluorene (spiro-OMeTAD)** used for solid-state dye-sensitized solar cells as well as an efficient HTM in the rapidly developing area of perovskite solar cells. In particular, the ionization potential of **spiro-OMeTAD** matches well with that of the light absorbers (perovskites or dye-sensitizers), and good contact at their interfaces is promoted by the remarkable glass forming properties of spiro-OMeTAD. These advantages make spiro-OMeTAD the most extensively studied organic HTM for hybrid organic-inorganic solar cells

[Flexible Electronics (2017) 1:2 ; doi:10.1038/s41528-017-0002-0]

The development of high-efficient silicon solar cells is, however, approaching its theoretical efficiency limit of 29.4%.



As a next step, the concept of silicon-based tandem solar cells is promising to break this limit. Stacking two solar cells on top of each other, the top cell — **with a high band gap** (**metal halide perovskite having ABX_3 crystal structure**) material — utilizes **high energy photons** while **the silicon bottom cell utilizes low energy photons**. Perovskite have a tunable band gap — the parameter that determines which part of the solar spectrum is utilized.



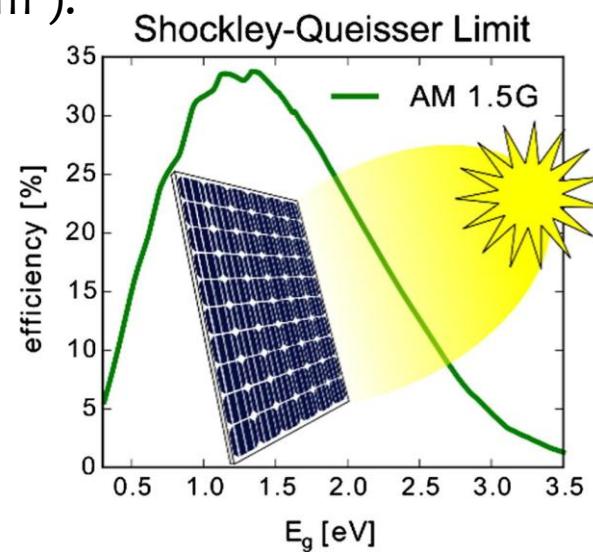
The Shockley-Queisser Limit

Shockley and Queisser, Journal of Applied Physics, Volume 32, pp. 510-519 (1961)

- The SQ limit was first calculated by [William Shockley](#) and [Hans-Joachim Queisser](#) at [Shockley Semiconductor](#) in 1961 based on theoretical conversion efficiency limit for single P-N junction crystalline silicon solar cells.
- The maximum [solar conversion efficiency](#) is around 33.7% assuming typical sunlight conditions ([AM 1.5 solar spectrum](#), 1.34 eV).
- That is, among all the sunlight power (about 1000 W/m²) falling on an ideal solar cell, only 33.7% of that could ever be turned into electricity (337 W/m²).

The limit of 33.7 % accounts to various other losses pertaining to solar cells:

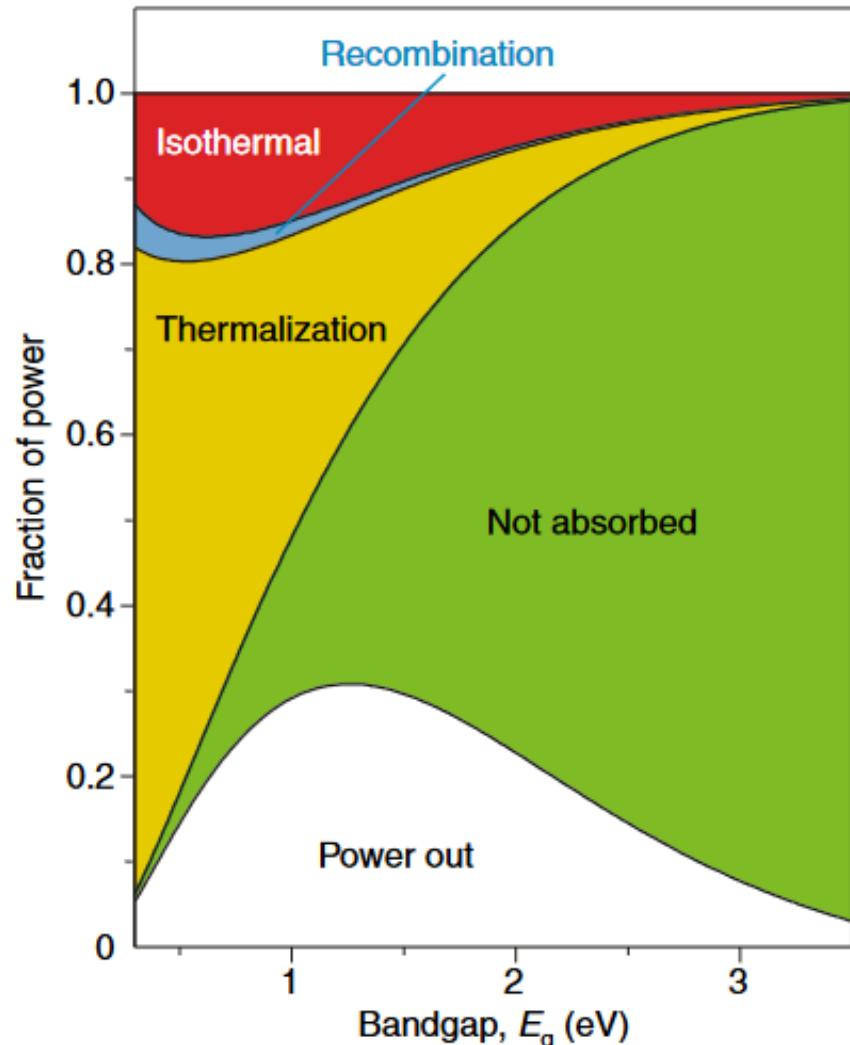
(1) Blackbody radiation, (2) Spectrum losses, and (3)
Recombination of exciton



The GaInP/GaAs tandem cell ($\eta = 32.8\%$) shows an efficiency well above that of the record for the individual cells ($\eta = 22.0\% / 29.1\%$).

A major breakthrough is the fact that perovskite/Si tandems have just recently significantly exceeded the record for the Si-only cell ($\eta = 29.2\%$ versus 26.7%).

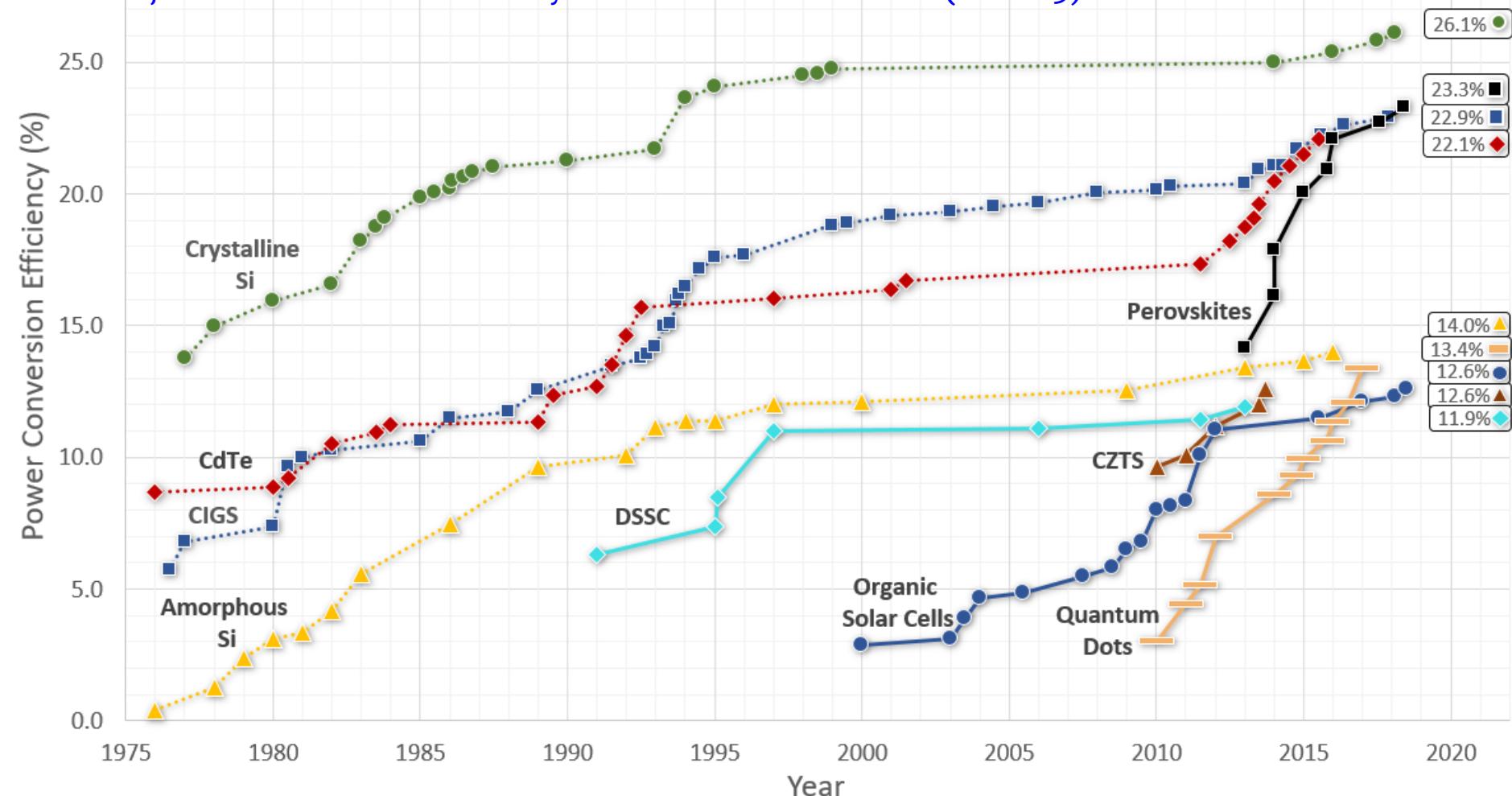
The Limitations of Silicon Solar Cells



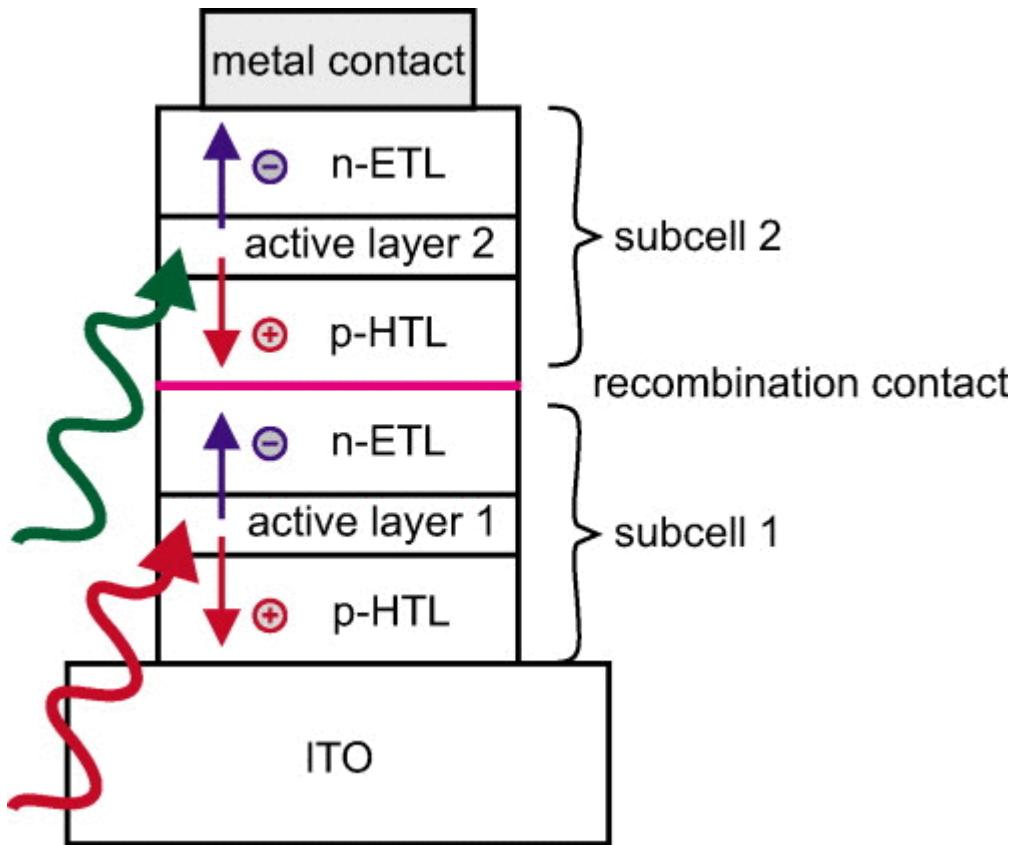
- **Optical:** Photons with energy lower than the bandgap are not absorbed. The higher the bandgap, the higher the amount of non-absorbed photons (~ 19% of the total losses).
- **Thermal:** Photons with an energy that exceeds the Bandgap ($E > E_g$) are absorbed. The generated carriers are thermalizing down to the band edge. The excess energy is released as heat to the solar cell (~ 33% of the total losses).
- **Electronic:** Loss due to radiative charge recombination, i.e. the pair recombines and, eventually, a photon is emitted. (~ 15% of the total losses).
- **Isothermal losses:** An additional electronic contribution due to the power dissipation along the band-edge (constant temperature of the carrier).

These losses result in about 68% of the total sunlight not being converted into electricity

Studies on perovskite solar cells have principally been on polycrystalline film power conversion efficiencies (Pc-PSCs). The record efficiency for Pc-PSCs, currently at 24.2% PCE, is still far from their theoretical Shockley–Queisser limit (SQL), which is ~30.5% PCE for a single-junction cell based on methylammonium lead triiodide (MAPbI₃).



Perovskite solar cells have increased in power conversion efficiency at a phenomenal rate compared to other types of photovoltaics.



Perovskite Solar Cell Durability

The durability of perovskite solar cells for long time usages is a concern. Some common standards for developing solar cells are as follows:

- Initially, a rule for any “commercial” solar cell was to maintain a power conversion efficiency of 10% for 10 years.
- Today, to realistically compete with crystalline-Si solar, a cell needs to last for 25 years in outdoor conditions to be marketable, and have similar efficiencies.
- According to the International Electrotechnical Commission's (IEC) standards, solar cells must perform well under non-laboratory conditions, such as in damp conditions i.e. 85% humidity at 85 degrees Celsius. They must withstand these for more than 1000 hours consistently.

Currently, perovskite solar cells still do not reach these standards. A recent review presents a detailed summary of various studies that have been done on perovskite stability. This includes a triple cation perovskite withstanding 85% humidity for 250 hours, and a methylammonium lead iodine (MAPbI_3) perovskite solar cell withstanding 55% humidity for 480 hours [[nt J Energy Res. 2021;1-17](#)].

Si-solar cells: Expensive to purify but cost-effective when volume is high

Perovskite solar cells: Solution processed with lower manufacturing cost.

26.6 % efficiency in single crystal Si cells

24.2% efficiency in stabilized perovskite solar cells.
Certified efficiency achieved ~22.5%

Cost

Efficiency

Durability

Si-Solar Cells ~ 25 yrs in outdoor condition

Longest reported perovskite stability ~ 1 yr

<https://www.ossila.com/pages/perovskite-solar-cell-degradation-causes>

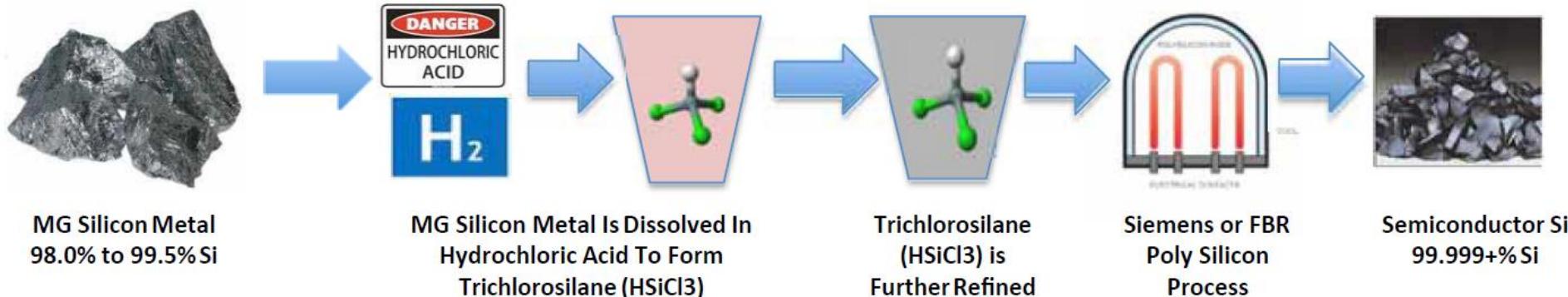
A bilayer conducting polymer structure for planar perovskite solar cells with over 1,400 hours of operational stability at elevated temperatures. [Nature Energy, 2022, 7, 144–152.]

For more details....

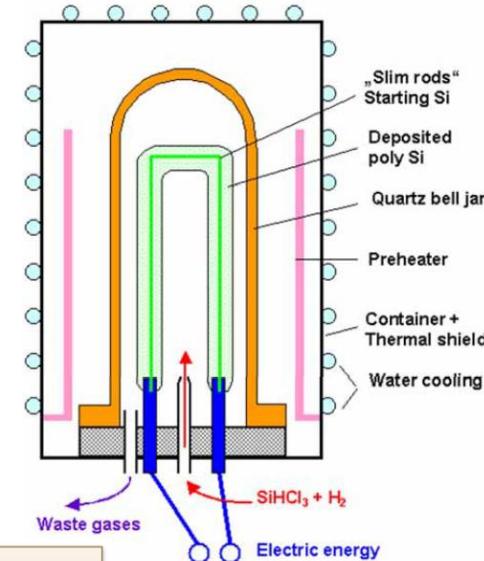
Promises and challenges of perovskite solar cells;

Science 2017; 358, Issue 6364, 739-744; DOI: 10.1126/science.aam6323

Si metal to Semiconductor grade Polysilicon

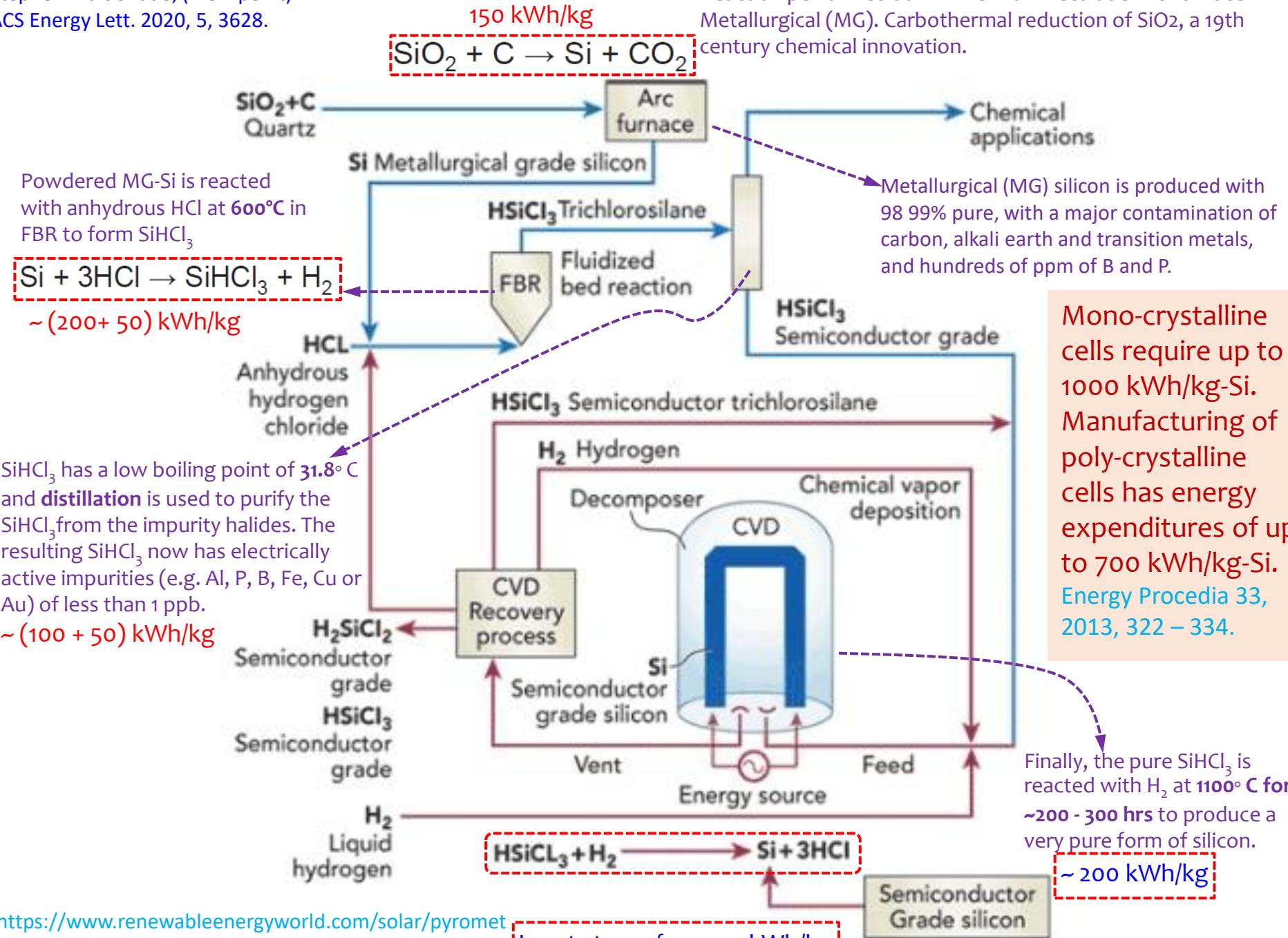


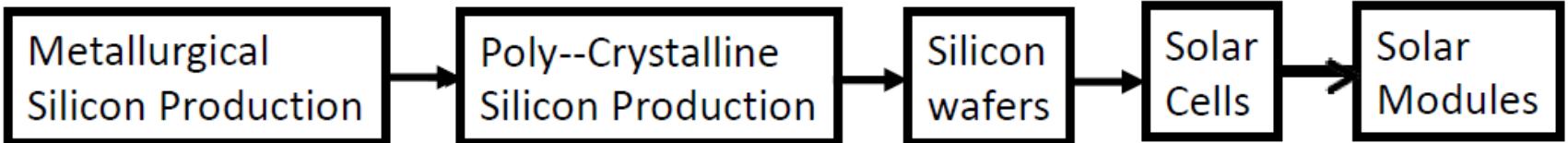
- Purify TCS in distillation columns
- Recover pure Si using Chemical Vapor Deposition (CVD)



Cold wall reactor, high energy consumption. TCS conversion per pass is around 15%, recycling and lower productivity

80% of the global polysilicon is produced using Siemens' process, developed in the 1950s.





IS SILICON PV GREEN ENERGY ?

Consider the following facts

- Solar PV manufacturing processes involve converting quartz to metallurgical grade silicon and then to polysilicon ingots which are sliced to form wafers
- Every ton of metallurgical grade silicon production results in 4 tons of silicon tetrachloride; **Material utilization efficiency is a mere 30%**
- 1 ton of crude silicon production results in 10 tons of CO₂; Purification process results in additional 45 tons of CO₂; for manufacturing in China, 70 g CO₂ is generated per kWh of electricity

Total energy expenditure for solar cell manufacturing

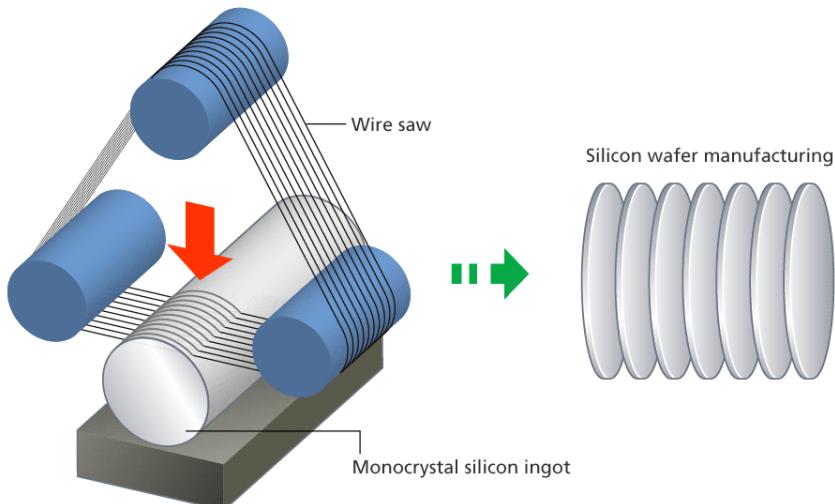
The total energy expenditure for solar cell manufacturing is the sum of the aforementioned processes. Mono-crystalline cells require up to 1000 kWh/kg-Si. Manufacturing of poly-crystalline cells has energy expenditures of up to 700 kWh/kg-Si.

Schematic of c-Si PV module supply chain



Silicon Solar Cell Manufacturing Process

www.cleanenergyreviews.info



Other Issues:

- Silicon production uses SF₆ (to clean the Siemens Reactor: **a potent GHG**), HF (to clean wafers and texture the surfaces), 1,1,1 trichloroethane (**a persistent pollutant**) and large quantities of strong acids.
- Conversion of ingots to wafers requires mechanical sawing, generating up to 10 % waste and a significant amount of fine silicon dust (inhalation hazard)
- Silver that is used for making panels at 5 % of current power demand will consume 50% of current silver produced.
- Little or no recycling of silicon in process waste or end of life panels

1,1,1 trichloroethane (TCA) remains a persistent pollutant at many sites and some of the daughter products that accumulate from intrinsic decay of TCA have been determined to be more toxic than the parent compound. [Water Research, 2011, 45, 2701-2723]

Table 3. Emissions form photovoltaic module and system.

Energy Procedia 33 (2013) 322 – 334

		SO ₂	NO _x	Particles	CO ₂	CH ₄	N ₂ O	Source
Emissions (kg/kW _p)	PV Module 1995/1998	5 - 5.5	4.5 - 5.3	No Info	2.7 - 3.8	No Info	No Info	[5, 6]
	Entire PV System 1998	1.9	1.8	0.11	971,000	1.6	0.0031	[3]

MAKING SILICON IS AN EXPENSIVE PROCESS

- High temperatures, invariably produced using electrical energy
- Long reaction times
- Several unit & Batch processes
- Large number of waste and by products
- Highly corrosive environment

Socio-Economic and Environmental Impacts of
Silicon Based Photovoltaic (PV) Technologies;
Energy Procedia 33 (2013) 322 – 334

Global capacity for solar grade silicon : ~ 0.5 million tons per annum

Minimum viable economic capacity : 10,000 tons per annum

Highly capital intensive : US \$1.5 million per ton of production

By contemporary standards of chemical manufacturing, the process for producing silicon is a highly complex process

Reduce



Reuse



Recycle

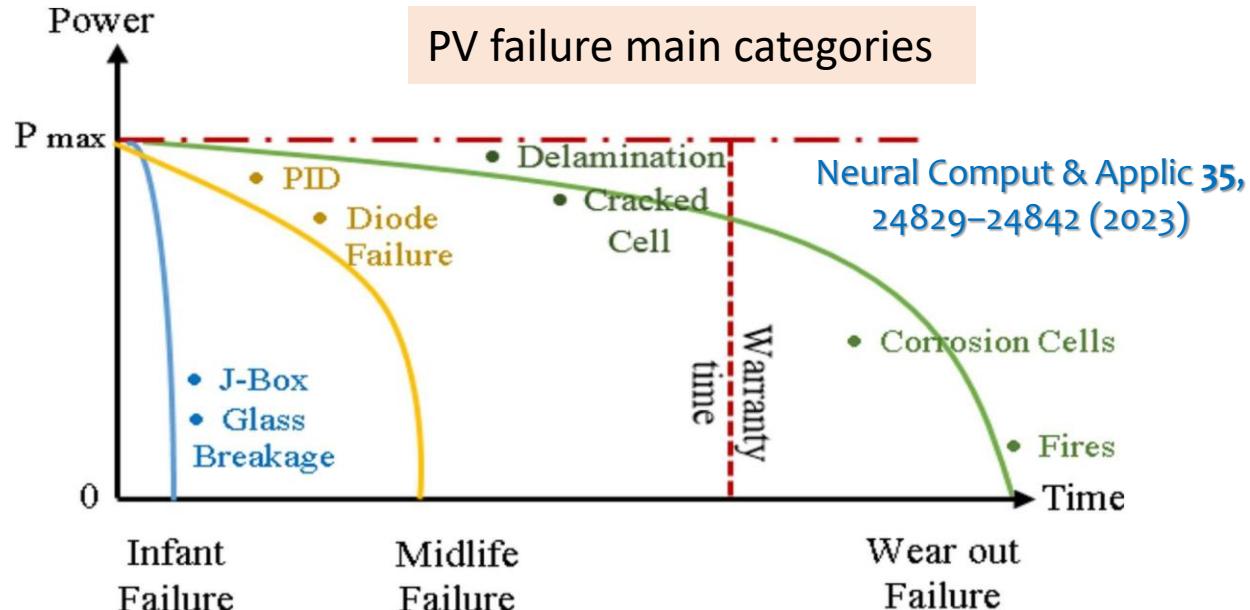


Dispose

Most preferred option

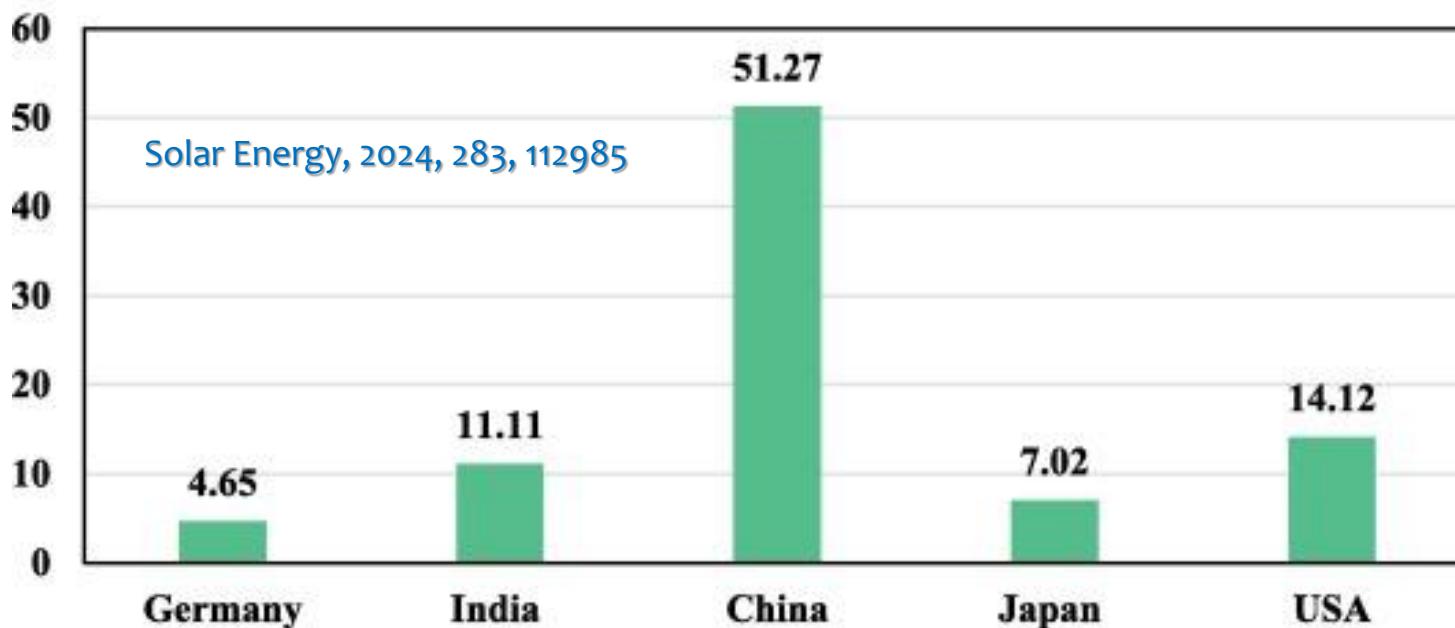


Least preferred option



Solar Energy, 2024, 283, 112985

PV waste in 2050 (Mt)



Hydrogen Energy

Sayam Sengupta,

S. Sivaram

[Amitava Das](#)

CH5106

Hydrogen energy involves the use of hydrogen and/or hydrogen-containing compounds to generate energy to be supplied to all practical usages for inclusive growth without compromising the social benefits (human well being), as well as economic competitiveness.

Modern Li-ion batteries have a maximum energy density of ~0.15 to 0.18 kWh per kg.

- Hydrogen: ~33 kWh per kg
- Li-ion: ~0.15 to 0.30 kWh per kg

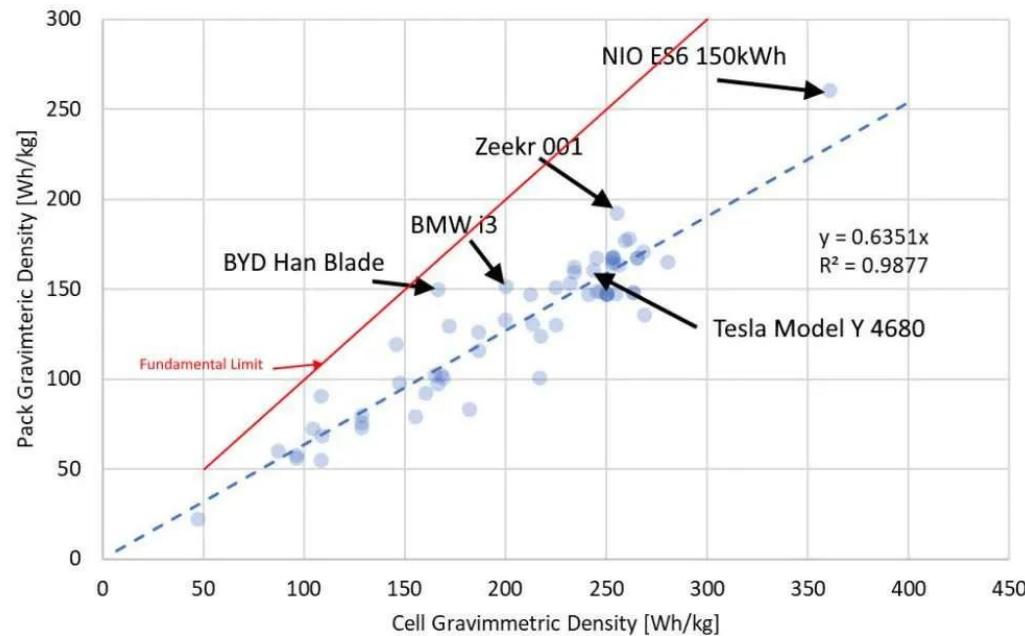
Needed battery mass to match 1 kg of H₂ energy storage:

$$\text{Mass} = \frac{33}{0.15 - 0.30} \approx 110 \text{ to } 220 \text{ kg}$$

- Lead-acid: ~0.037 kWh per kg (roughly)

$$\text{Mass} = \frac{33}{0.037} \approx 892 \text{ kg}$$

<https://www.batterydesign.net/battery-pack-density-fundamental-limit/>



Pack gravimetric energy density: A measure of a battery pack's total energy capacity per unit of weight (Wh/kg cap Wh/kg).

Cell gravimetric energy density: A measure of the energy per unit of weight for a single cell (Wh/kg cap Wh/kg).

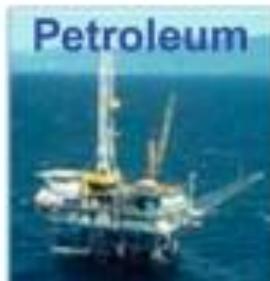
Toward Zero C Emissions



10 atoms of C
for 1 atom of H₂



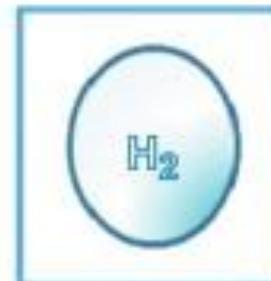
2 atoms of C
for 1 atom of H₂



1 atom of C
for 2 atoms of H₂

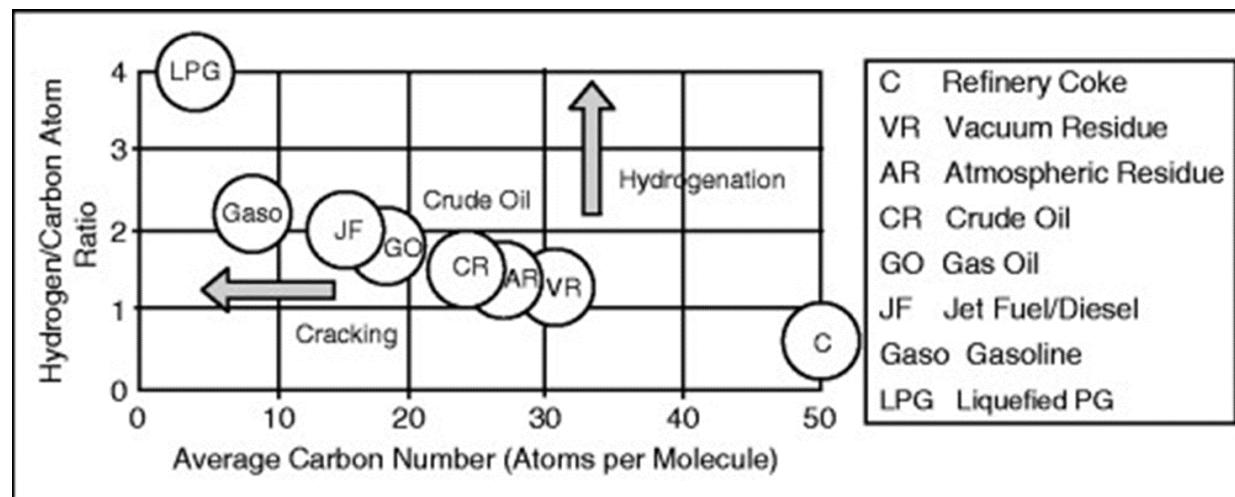


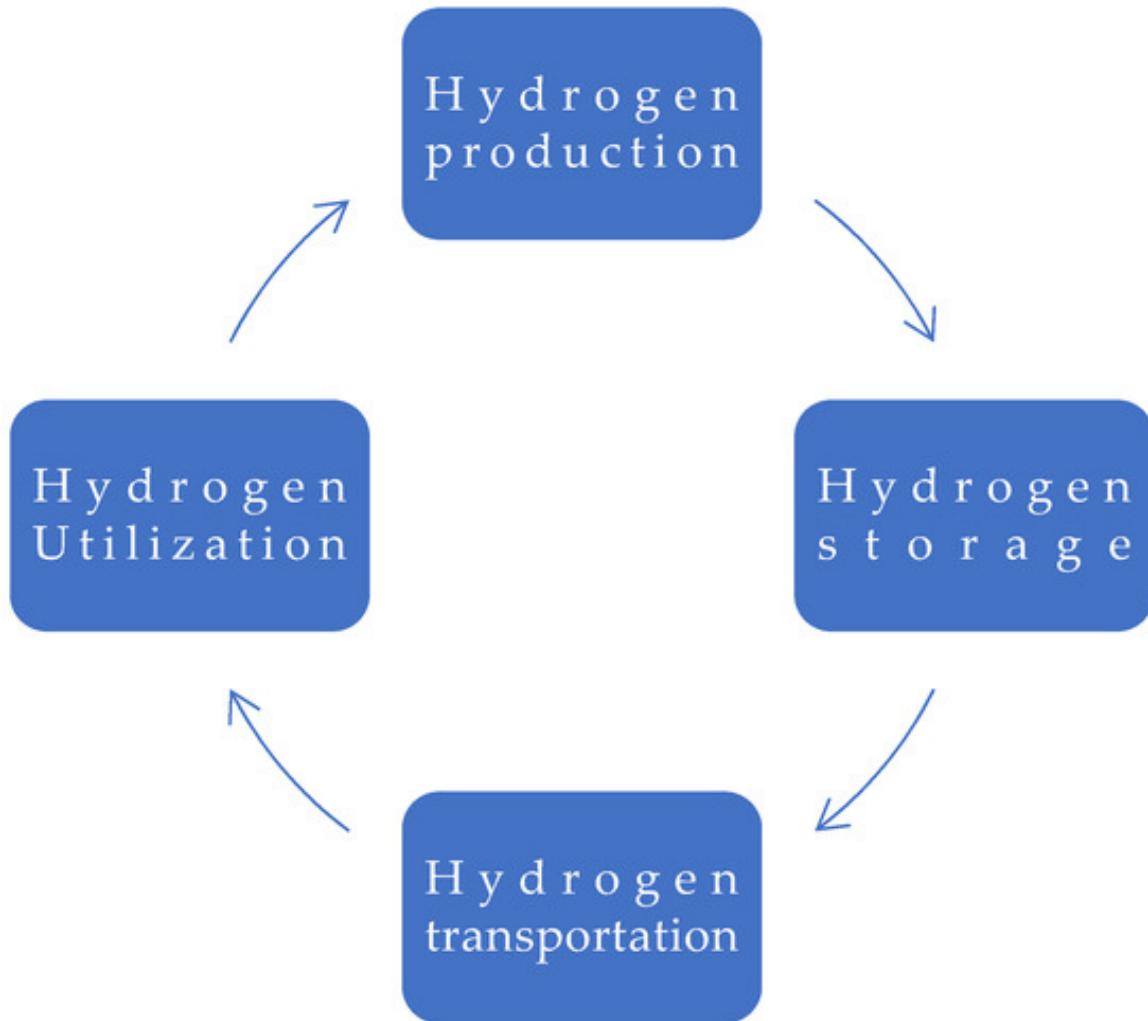
1 atoms of C
for 4 atoms of H₂



0 atoms of C
for 2 atoms of H₂

The ratio of the atom numbers of carbon and hydrogen





The **ideal storage medium** should allow high volumetric and gravimetric energy densities, quick uptake and release of fuel, operation at room temperatures and atmospheric pressure, safe use, and balanced cost-effectiveness.

How is hydrogen stored?

Physical-based

Compressed Gas



Cold/Cryo Compressed



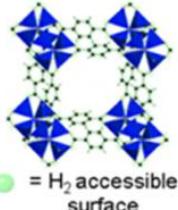
Liquid H₂



Material-based

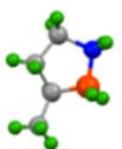
Adsorbent

Ex. MOF-5



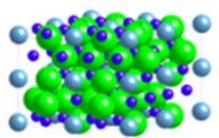
Liquid organic

Ex. BN-methyl cyclopentane



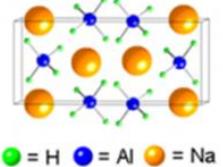
Interstitial hydride

Ex. LaNi₅H₆



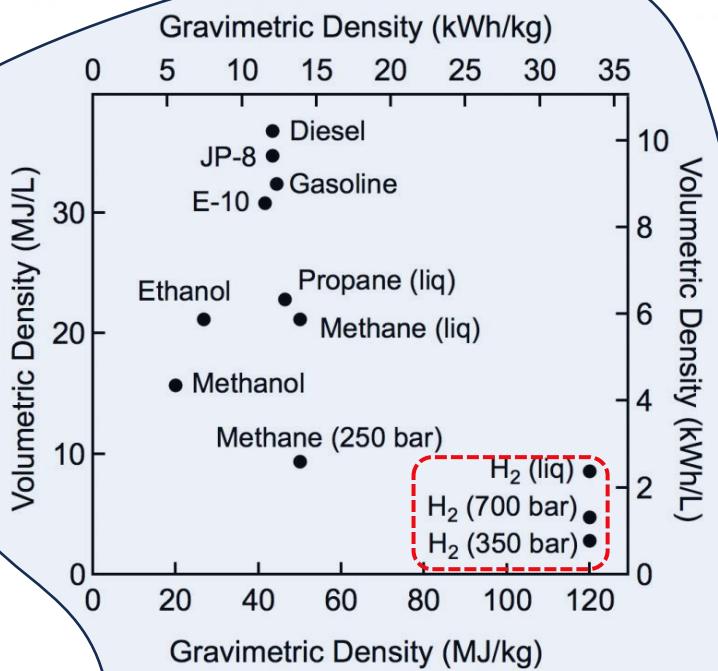
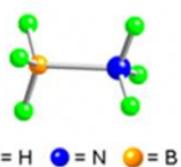
Complex hydride

Ex. NaAlH₄



Chemical hydrogen

Ex. NH₃BH₃



Comparison of specific energy (energy per mass or gravimetric density) and energy density (energy per volume or volumetric density) for several fuels based on lower heating values.

The Hydrogen and Fuel Cell Technologies Office (HFTO) is pursuing two strategic pathways: near-term and long-term solutions. The near-term approach focuses on compressed gas storage using advanced fiber-reinforced pressure vessels (up to 700 bar) with emphasis on cost reduction. The long-term approach targets (1) cold or cryo-compressed hydrogen storage with higher density and insulated vessels, and (2) materials-based storage technologies such as sorbents, chemical hydrides, and metal hydrides to meet DOE targets.

Targets are set with stakeholder input to ensure competitiveness and guide RD&D efforts, shaping HFTO's activity portfolio. Examples include the following.

[efaidnbmnnibpcajpcglclefindmkaj/https://www.energy.gov/sites/default/files/2024-05/hfto-mypp-executive-summary.pdf](https://www.energy.gov/sites/default/files/2024-05/hfto-mypp-executive-summary.pdf)

Clean H₂ production:

- \$2/kg by 2026; \$1/kg by 2031

Electrolyzer systems (low temperature):

- 2026: \$250/kW, 65% efficiency, 80,000-hour durability

Electrolyzer systems (high temperature):

- 2026: \$500/kW, 76% efficiency, 40,000-hour durability

H₂ dispensed for heavy-duty transportation:

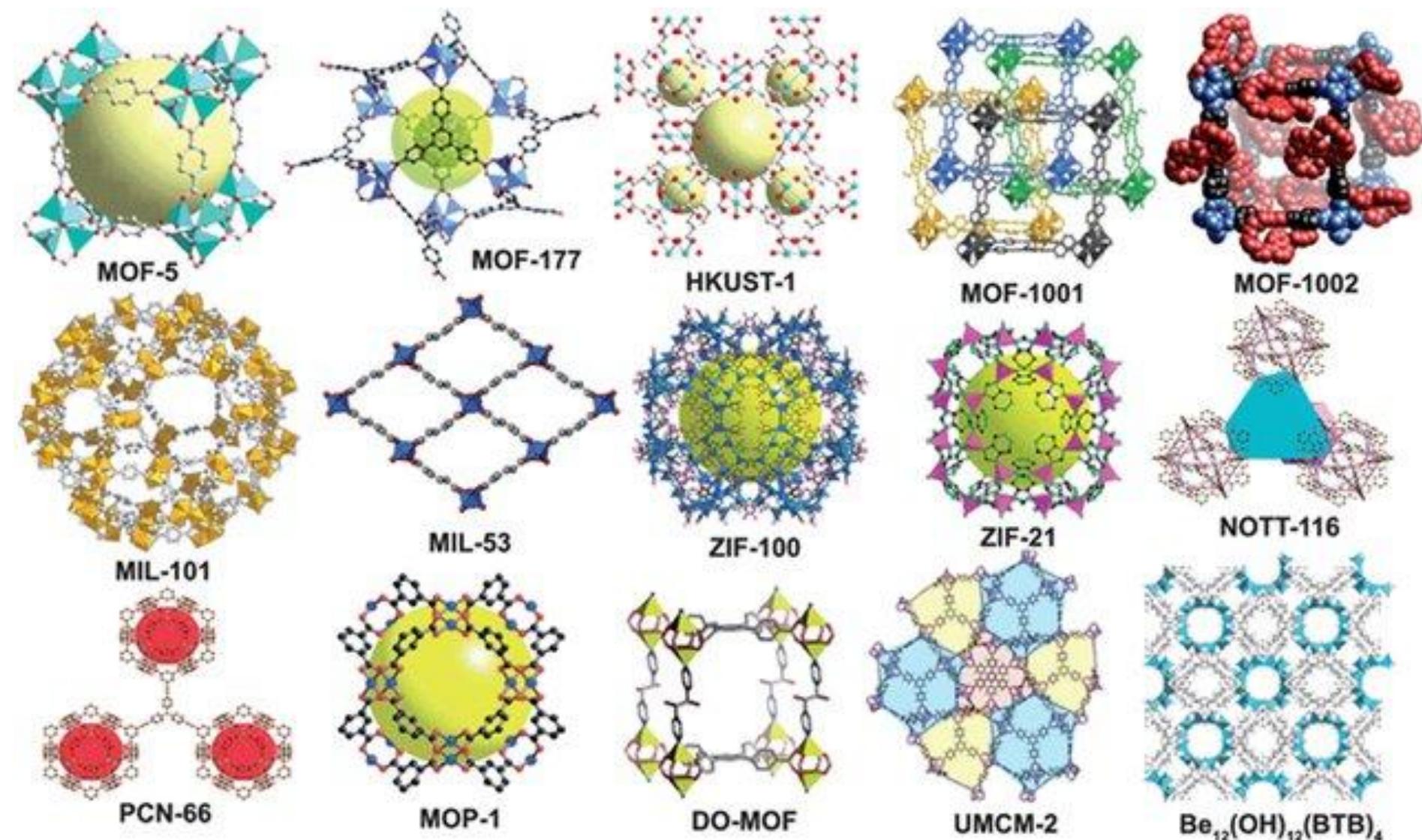
- 2028: <\$7/kg

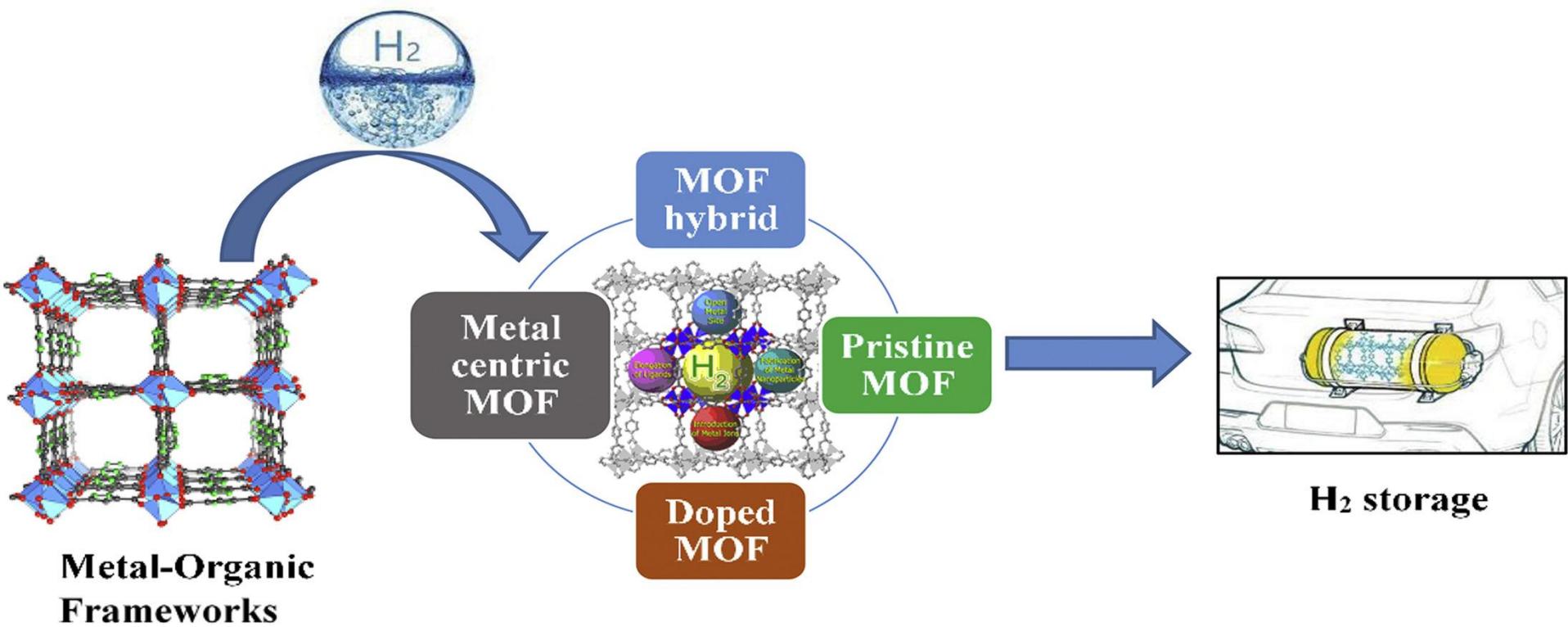
Fuel cell manufacturing for heavy-duty transportation:

- 2030: 20,000 stacks/year (single manufacturing system)

Fuel cell systems for heavy-duty transportation:

- 2030: \$80/kW, 25,000-hour durability





Challenges associated with MOF-based H₂ storage:

The hydrogen storage capacity is 7.1 wt.% at 77 K and 40 bar; 10 wt.% at 100 bar; corresponding to 66 g·l⁻¹. The fueling process is quite fast.

Issues: Low thermal conductivity of (0.3 W/(mK)) of MOFs represents an additional challenge for the thermal management in the design of MOF-based storage systems.

The actual 2025 DOE hydrogen storage objectives is a part of the broader U.S. DRIVE initiative, set standards for the complete H₂ storage system. The targets address the need for a balanced approach to storage, considering gravimetric capacity (weight), volumetric capacity (volume), and operational conditions.

<https://www.energy.gov/eere/fuelcells/doe-technical-targets-onboard-hydrogen-storage-light-duty-vehicles#:~:text=Useful%20constants>

For technological applications, rapid kinetics and full reversibility enable short refuelling times and high cycle life, and so exploration into physisorption in materials is an important area. [Journal of Alloys and Compounds 827 \(2020\) 153548](#)

Liquid hydrogen is the most conceptually simple means of hydrogen storage; however, the complexity and cost associated with the extremely low temperature (20 K) required for hydrogen liquefaction has prompted the consideration of other liquid carriers with moderate storage conditions.

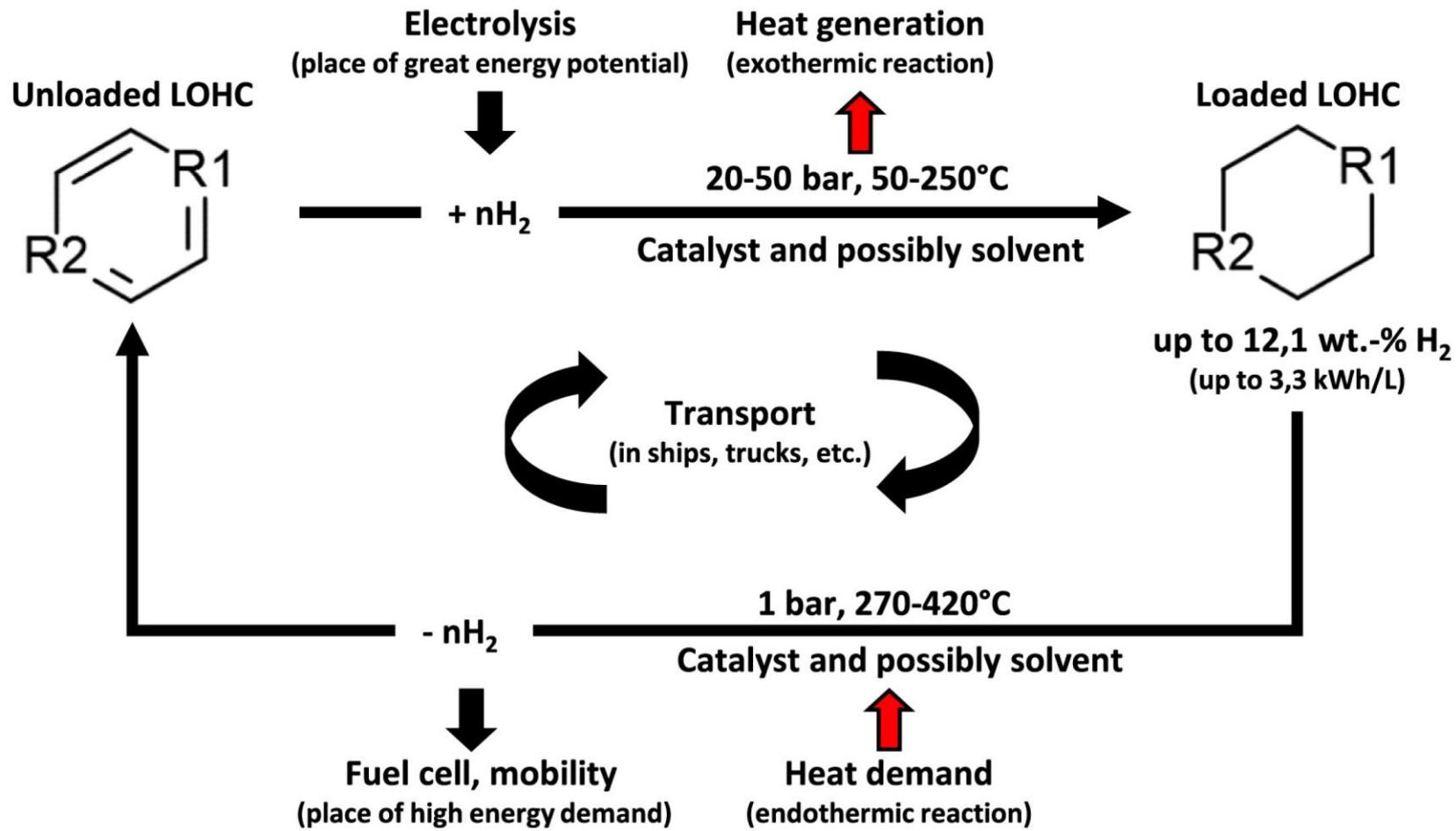
Most attention has been given to two carriers in particular:

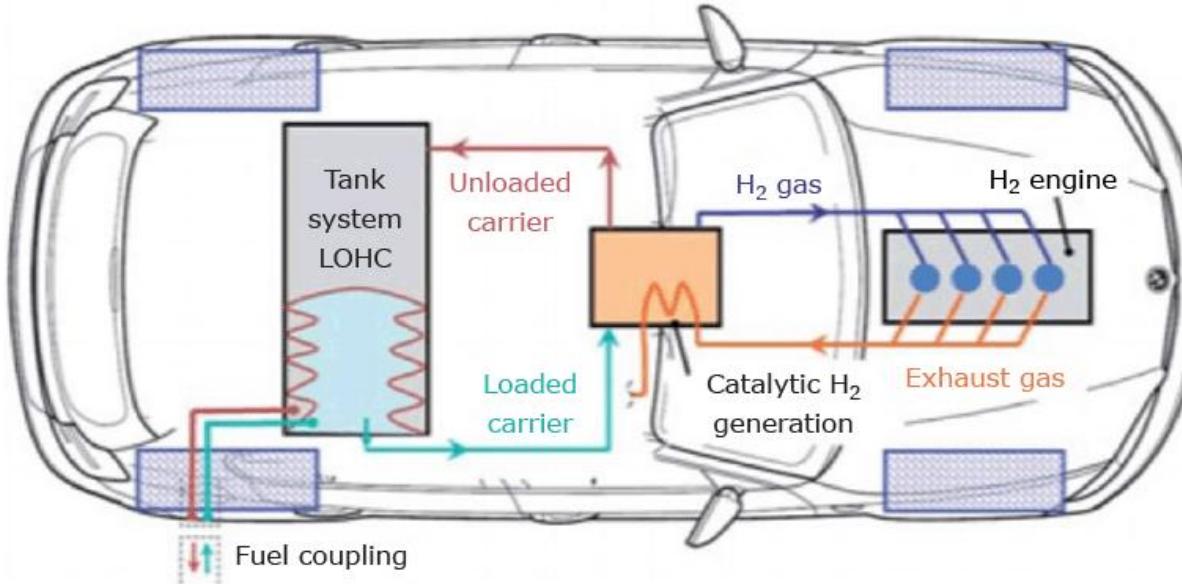
Liquid organic hydrogen carriers (LOHCs) and ammonia. Both have moderate storage requirements and storage costs compared to liquid hydrogen. This has led to the active development of hydrogen supply chains based on conversion to these carriers.

David Milstein & Coworkers, Nature Commun. 2015, 6:6859; DOI: 10.1038/ncomms7859;

Chem. Eur. J. 2020, 26, 15487 – 15490

Päivi T. Aakko-Saksa & Coworkers; Journal of Power Sources, 396 (2018) 803–823

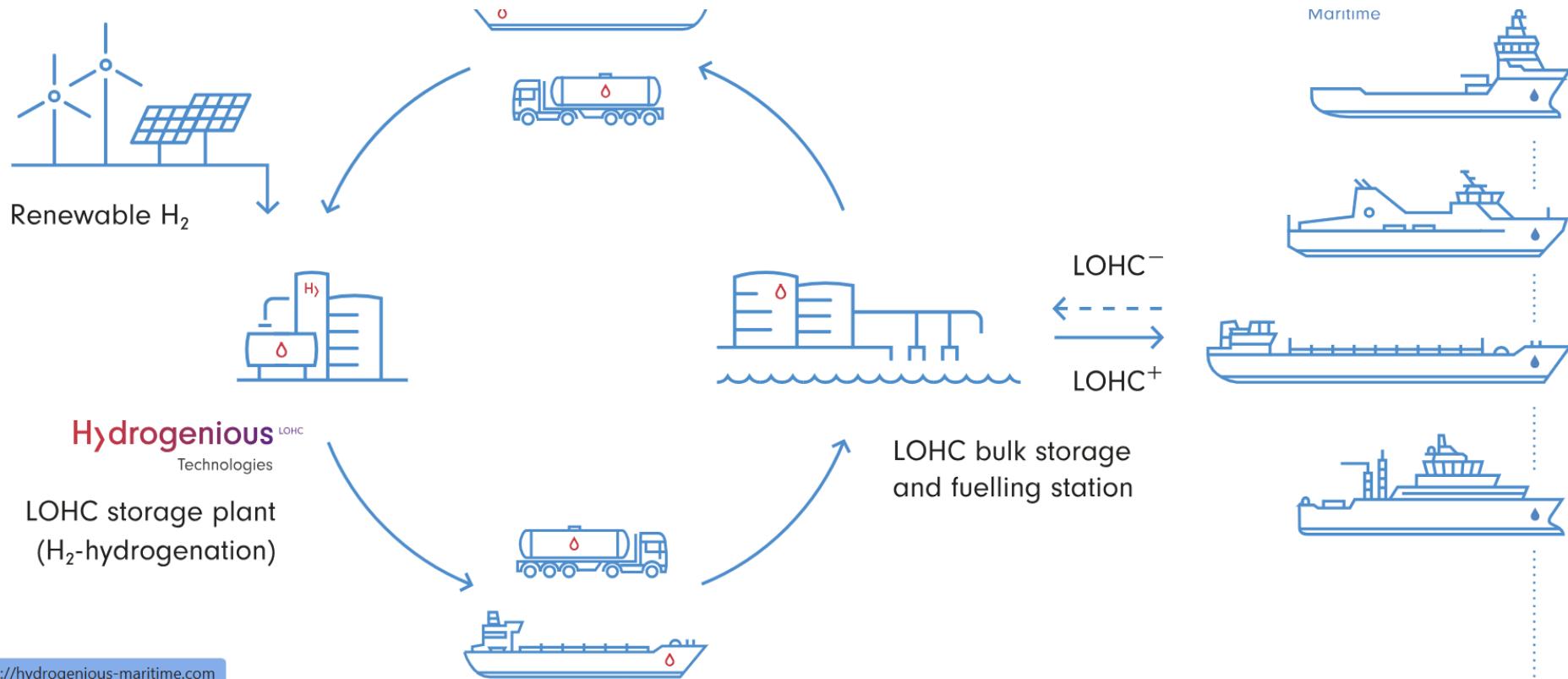




Johnson Matthey Technol. Rev., 2022, 66, (3), 259–270

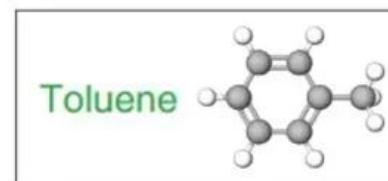
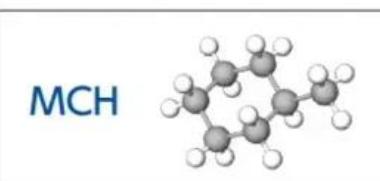
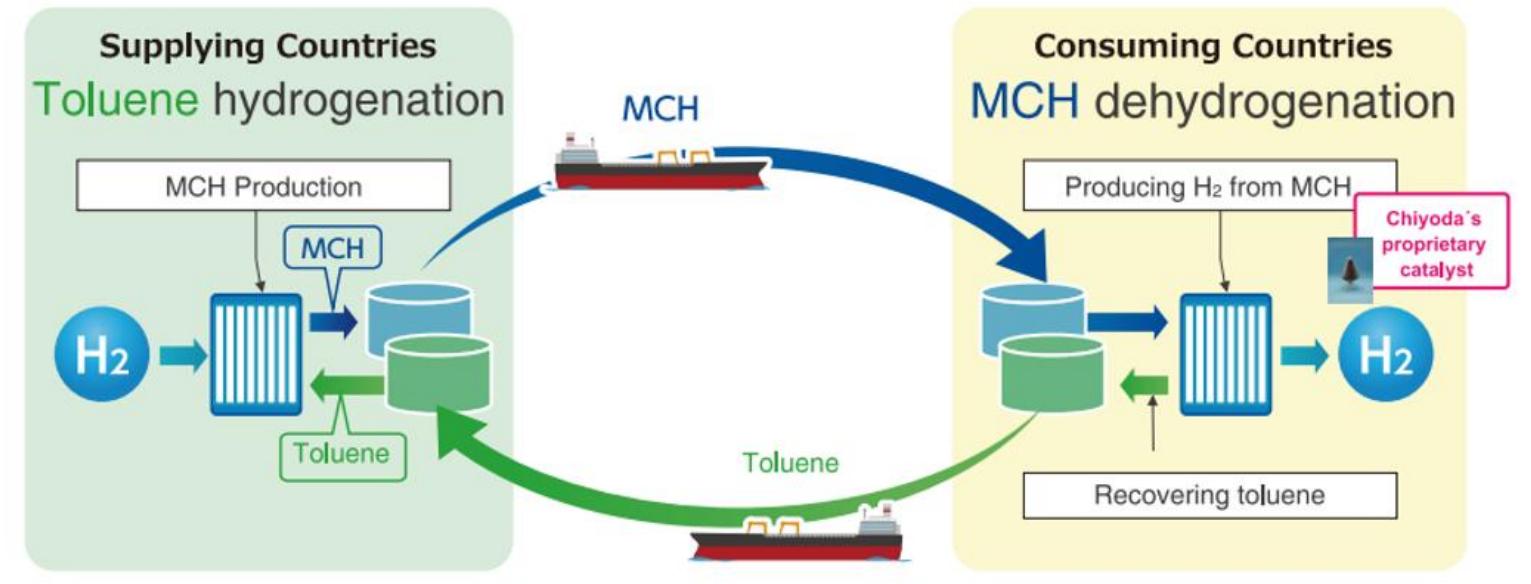
Advantageously, onboard storage of hydrogen in the LOHC would resemble that of gasoline and diesel (liquid state of the LOHC at ambient pressures), which is widely understood, and the safety hazards of storing high-pressure hydrogen are removed. Moreover, a range of 500 km is reportedly achievable using 100 lit of NEC loaded with hydrogen (equivalent to 5 kg of hydrogen) as the LOHC.

Hyundai Motor Company, South Korea, has recently announced plans to develop an onboard LOHC storage technology. This encompasses a partnership with **Hydrogenious LOHC Technologies GmbH**, Germany, which will supply dibenzyl toluene to be used as the LOHC. Initially, the technology will be introduced in South Korea, before being extended to the European market. The development of LOHC-compatible automobiles is expected to raise the profile of the technology as an important tool in the transition to the hydrogen economy [Johnson Matthey Technol. Rev., 2022, 66, (3), 259–270].

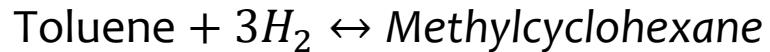


<https://hydrogenious.net/how/>

Chiyoda Corporation

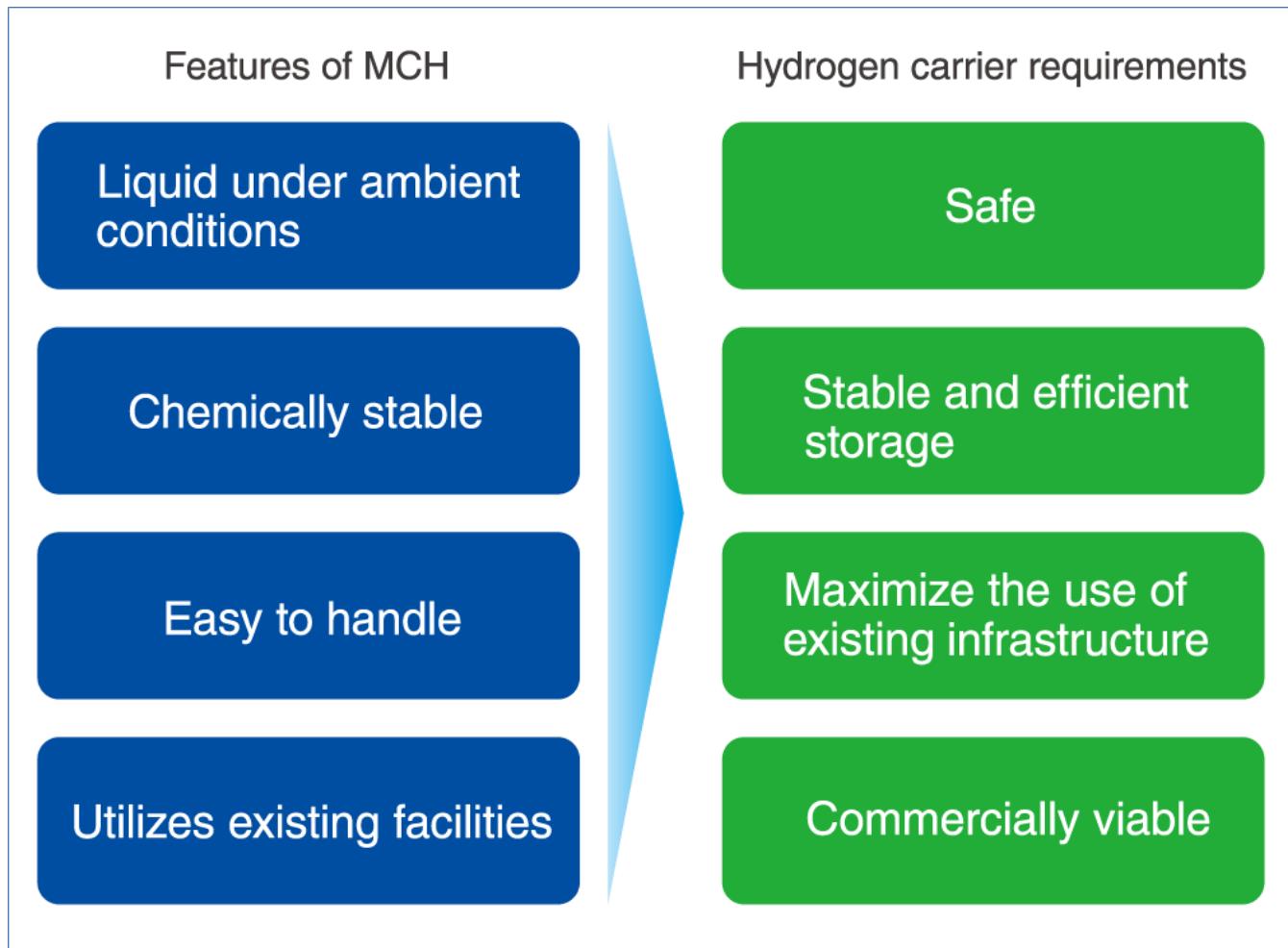


Methylcyclohexane (MCH) is commonly used as a hydrogen carrier in LOHC technology. It stores hydrogen chemically by hydrogenating toluene to form MCH:



https://www.chiyodacorp.com/en/purposesstory/co-creation/spera-hydrogen/?utm_source=chatgpt.com

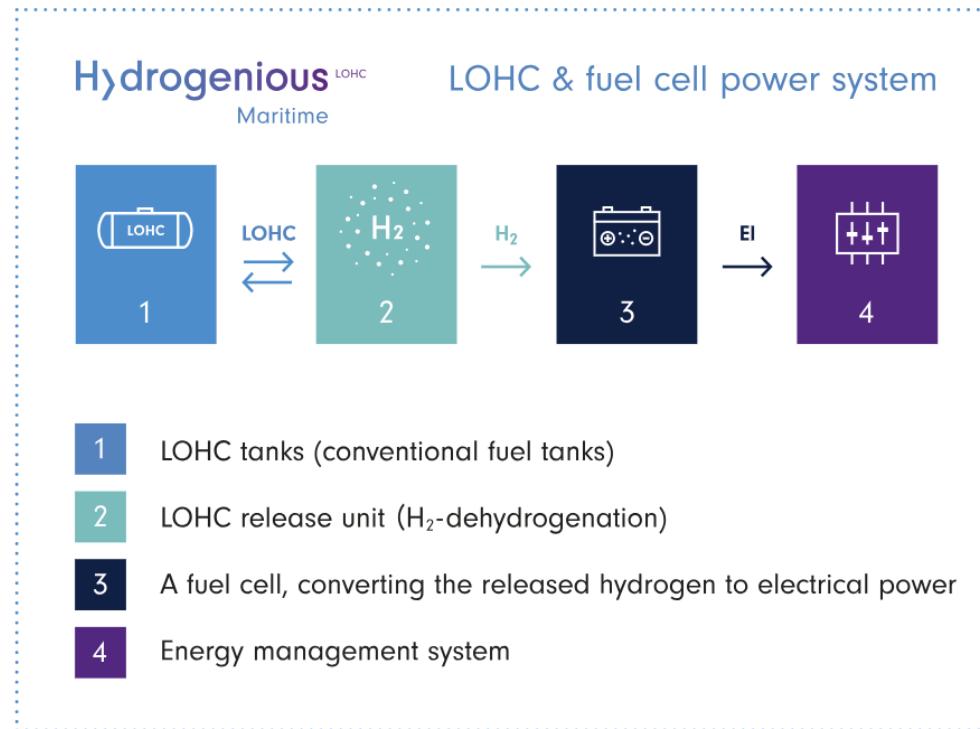
Chiyoda has developed technology to safely and efficiently store and transport hydrogen using Methylcyclohexane (MCH) as a Liquid Organic Hydrogen Carrier (LOHC) and termed it the ‘SPERA Hydrogen System’ (after “Spera” : Latin for “Hope”).



Where most commercial / pilot activity is focused (2025)

- **Germany / EU:** multiple demos and funded projects (TransHyDE, One Reactor, HyScale, etc.). [Hydrogenious LOHC Technologies+2](#) [Hydrogenious LOHC Technologies+2](#)
- **Japan:** Chiyoda + industrial partnerships pushing SPERA (MCH) for import/export chains and domestic supply. [Chiyoda Corporation](#)
- **Startups & new entrants:** Ayrton Energy (e-LOHC), Honeywell/ENEOS collaborations, and other private investments target commercialization & localized pilots.
- A position-paper states: “Hydrogen carrier technologies—including LOHCs already have a high technology readiness level (TRL 7 or higher as defined by the International Energy Agency/IEA) of the full value chain including hydrogen conversion and reconversion.” [ess.honeywell.com](#)
- The EU’s H2020 call for LOHCs specified: technology starting at TRL 4 and expected to reach **TRL 6** at the end of the project (for demonstration of distribution/storage chain) in the given timeframe. [CORDIS](#)
- According to a recent article: LOHC technology “is being commercialised by Hydrogenious LOHC Technologies ... Having completed the technological proof of concept for LOHC...” [mission-innovation.net](#)

“LOHC has reached pilot and demonstration stages for mobility-oriented infrastructure (refueling stations, LOHC transport units and maritime demos), but — as of the latest public records (through 2025) — **no commercial in-service vehicle fleet** has been publicly documented using an onboard LOHC system.



Liquid Organic Hydrogen Carriers are an advanced hydrogen storage technology that utilizes reversible chemical processes to store and release hydrogen. Through hydrogenation, hydrogen molecules are chemically bound to LOHC compounds, significantly enhancing gravimetric and volumetric storage capacities. When needed, hydrogen is released via a dehydrogenation process. Ideal LOHCs are liquid at ambient conditions, safe, cost-effective, and non-toxic, simplifying handling and transportation. Dehydrogenation of LOHCs is normally carried out at temperatures greater than hydrogenation with materials such as perhydro-dibenzyltoluene usually dehydrogenating around a temperature of about 300 °C, while hydrogenation occurs at lower temperatures (Decreasing the dehydrogenation temperature makes it feasible to integrate with low-temperature waste heat and makes energy efficiency better.

[Renew. Sustain. Energy Rev. 2021, 135, 110171](#)

Heat
 $T = 150\text{--}300^\circ\text{C}$
 $\approx -9 \text{ kWh}_{\text{th}}/\text{kg H}_2$

9 H₂

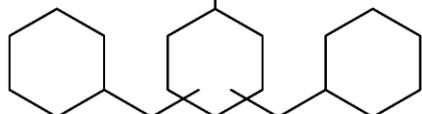
Dibenzyl-toluene as an organic liquid hydrogen carrier (LOHC) molecule.
Materials 2020, 13, 277; doi:10.3390/ma13020277

H₂-Storage
CATALYTIC HYDROGENATION

$P > 20 \text{ bar}$

LOHC⁺ (18H-DBT)

Perhydro-Dibenzyltoluene



$T_{\text{boil}} = \text{ca. } 370^\circ\text{C}$
(1 atm)

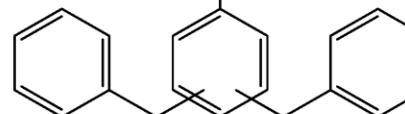
$\approx 16.1 \text{ kg LOHC}^+/\text{kg H}_2$

$\approx 17.5 \text{ L LOHC}^+/\text{kg H}_2$



LOHC⁻ (0H-DBT)

Dibenzyltoluene



$T_{\text{boil}} = \text{ca. } 390^\circ\text{C}$
(1 atm)

Multi phase
reaction

$P < 5 \text{ bar}$

H₂-Release
CATALYTIC DEHYDROGENATION

Heat
 $T = 250\text{--}320^\circ\text{C}$
 $\approx +9 \text{ kWh}_{\text{th}}/\text{kg H}_2$

9 H₂

Dibenzyl and benzyl toluenes were introduced commercially by German company Hydrogenious GmbH (<http://www.hydrogenious.net>). In Japan, Chiyoda Corporation (www.chiyodacorp.com) has demonstrated the use of the toluene LOHC system, called SPERA.

The strategy with LOHCs is to hydrogenate an organic compound to store hydrogen and dehydrogenate it when hydrogen is needed.

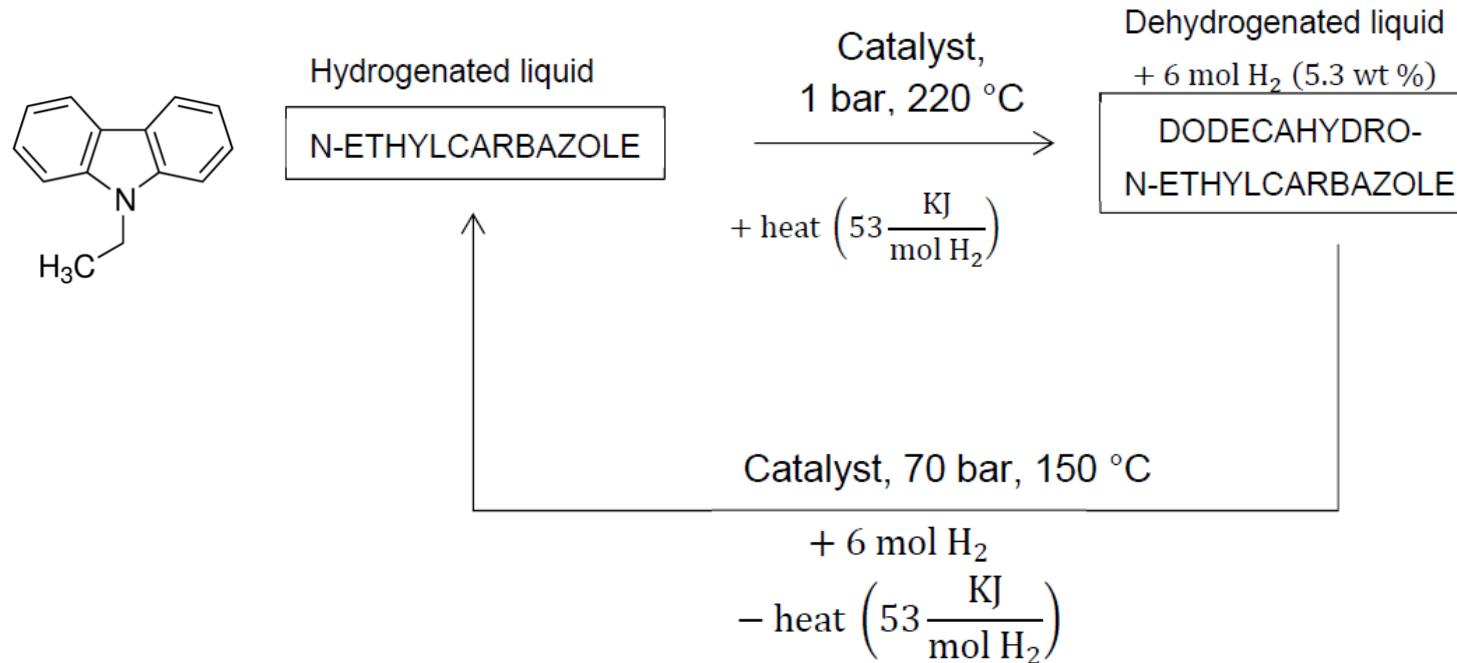


Figure 5. N-ethylcarbazole hydrogen uptake and release. [164].

The price of these precious metals is a major cost driver, and the monetary and environmental costs associated with the extraction of those metals are also significant. Development of stable dehydrogenation catalysts is necessary for decentralized use.

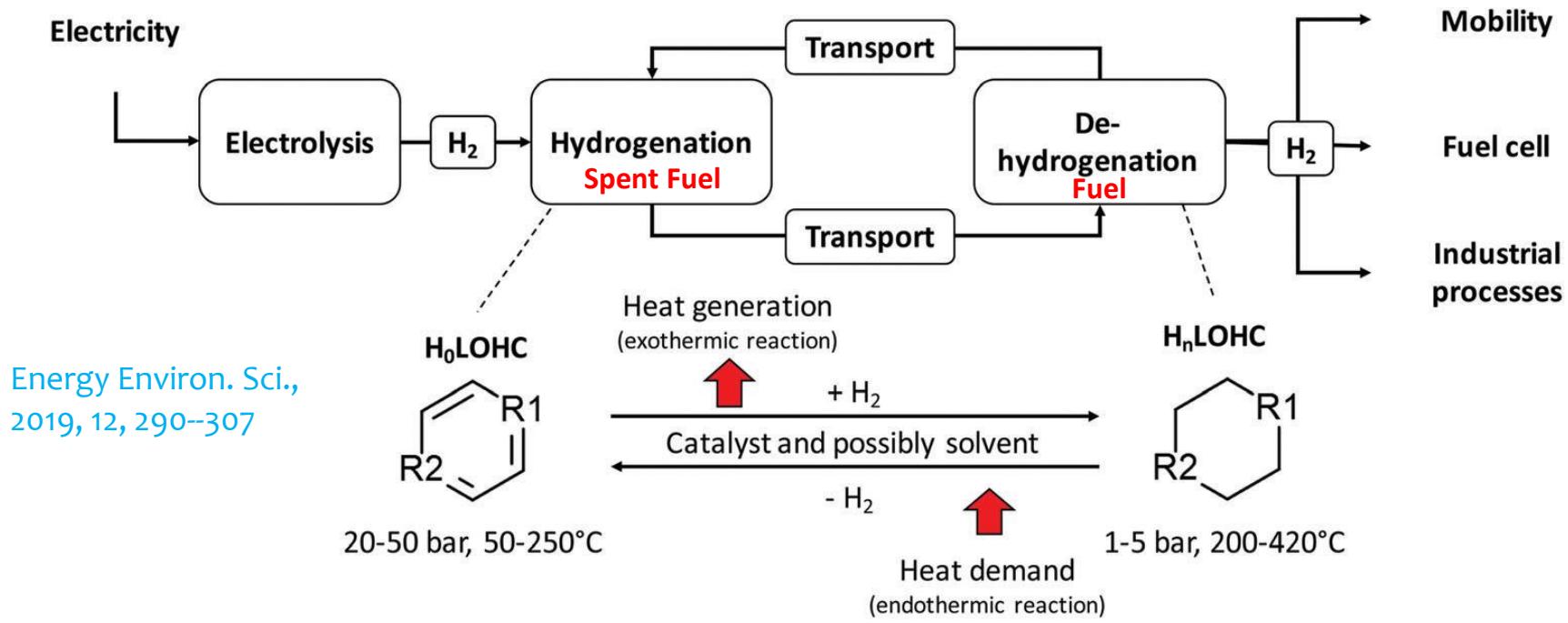
Dehydrogenation of this LOHC involves a significant amount of heat, nearly 60% of the gravimetric energy density of diesel fuel. Therefore, hydrogenation and dehydrogenation of LOHC are more suitable for applications where heat can be conveniently utilized or supplied (e.g. Fuel Cell application) Materials 2019, 12, 1973; doi:10.3390/ma12121973

LOHCs are at **pilot** → **early commercial** stage in 2025. Demonstrations and medium-scale plants exist, major industrial players (Chiyoda, Hydrogenious and several startups) are running pilots or deploying permit-approved systems, and new entrants/partnerships are pushing e-LOHC and scale-up. LOHCs remain promising for long-distance transport and stationary storage, but round-trip energy losses, catalyst & heat management, and system economics still limit widespread on-board vehicle use.

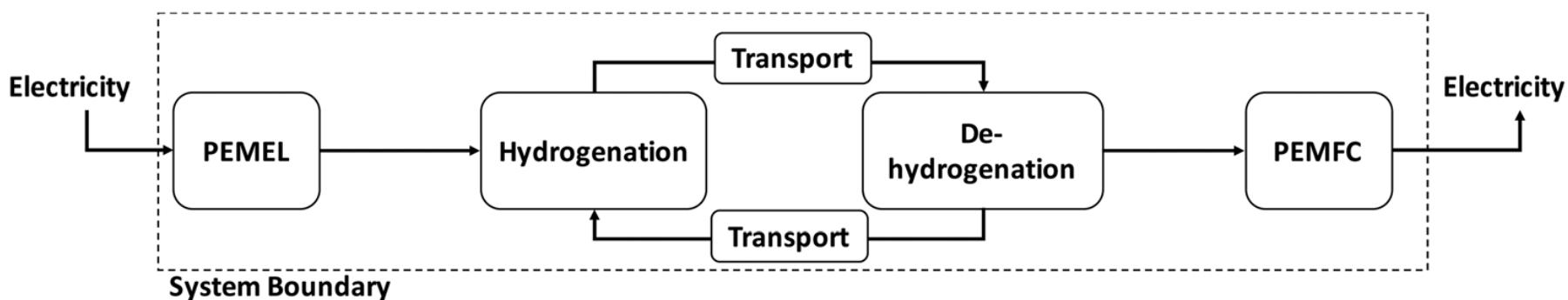
What's technically matured (2025)

Two LOHC families dominate:

- **MCH / toluene (SPERA)** — championed by Chiyoda (Japan). Well-demonstrated hydrogenation/dehydrogenation chain. [Chiyoda Corporation](#)
- **Hydrogenated dibenzyltoluene / dibenzyltoluene (DBT)** — used by Hydrogenious and partners; good thermal and handling properties for long-term storage/transport.



LOHC storage and transport concept ($H_0\text{LOHC}$: unloaded LOHC; $H_n\text{LOHC}$: loaded LOHC)



Flow diagram and system boundaries of the process chain (PEMEL: Polymer Electrolyte Membrane Electrolysis, PEMFC: Polymer Electrolyte Fuel Cell).
Process starts with electricity provided by renewable sources of energy and ends again with “green” electricity provided at another place and at another time.

Chemical Hydrogen:

The term chemical hydrogen is used to describe the strategy of storing hydrogen by synthesizing molecules that contain hydrogen (e.g. CH₄, NH₃)

- Ammonia can be liquefied at room temperature at pressures of 8-10 bar and stored in a similar manner to propane.
- Although it is toxic, its smell can be detected even at safe concentration levels (< 1 ppm).
- Ammonia is actually considered nonflammable when being transported.
- Ammonia is the second most widely produced commodity chemical in the world (second to sulfuric acid), and its worldwide distribution system is well established.
- For ammonia, infrastructure already exists.
- It contains 17% hydrogen by weight, which can be extracted via thermal catalytic decomposition or electro-oxidation. Alternatively, ammonia may be oxidized directly in fuel cells without the need for a separate reactor.
- Ammonia's energy density is comparable to that of compressed natural gas (CNG) and methanol, but lower than gasoline and liquefied propane gas (LPG).
- The life cycle production cost of energy from ammonia is estimated at US\$ 1.2/kWh compared to US\$ 3.8/kWh for methanol and US\$ 25.4/kWh for hydrogen.

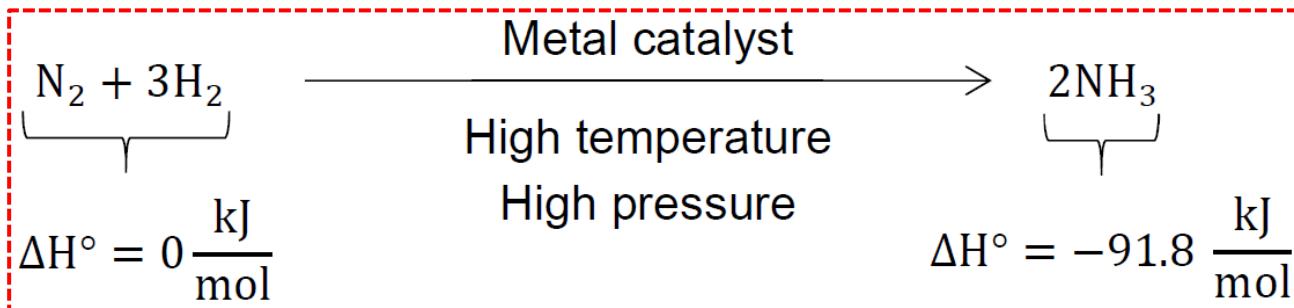
NH₃ had a worldwide production of 150 million metric tons in 2023, making it the second-highest-produced chemical commodity after sulfuric acid (H₂SO₄).

Gray or Brown NH₃: The Haber-Bosch process, responsible for nearly all of the world's 180 million t of annual ammonia production, reacts hydrogen and atmospheric nitrogen. The hydrogen often comes from the steam reformation of methane, a process that emits CO₂.

Blue NH₃: Blue ammonia is conventional ammonia with CO₂ has been captured and stored, reducing climate impact compared with gray ammonia. Many fertilizer makers have embarked on such projects in recent years.

Green NH₃: Green ammonia is made with hydrogen that comes from water electrolysis powered by alternative energy. Projects abound, though most are on a modest scale of tens of thousands of tons, an order of magnitude smaller than a typical ammonia plant. A massive project in Saudi Arabia, however, aims to make more than 1 million metric tons of ammonia per year.

Turquoise NH₃: This process uses pyrolysis to convert methane into pure carbon and hydrogen, which is reacted with N₂ to make ammonia. The industry thinks of turquoise ammonia as somewhere between green and blue. A prominent project is Monolith Materials' carbon black plant in Nebraska.



The energy density of liquid ammonia (17.6 wt %, 11.5 MJ/L) is marginally better than that of liquid hydrogen. A lower vapor pressure of ammonia (9.2 bar at 25 C) significantly simplifies the tank design. **Materials 2019, 12, 1973**

Similar to methane, ammonia utilization is more difficult than pure hydrogen. Solid oxide fuel cells are the most likely route for the use ammonia in fuel cells, but these fuel cells still have durability issues.

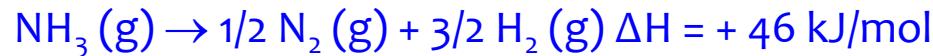
Is ammonia the fuel of the future?

Industry sees the agricultural chemical as a convenient means to transport hydrogen by [Alexander H. Tullo; March 8, 2021 @ C&EN](#) | A version of this story appeared in [Volume 99, Issue 8](#)

“Up to this point, we have made a business by selling the nitrogen value of the molecule. What’s really exciting about this is now there is an opportunity and a market that values the hydrogen portion of the molecule.”

AMMONIA DECOMPOSITION:

Ammonia decomposition (cracking) is simply the reverse of the synthesis reaction.



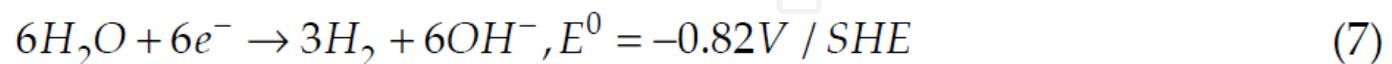
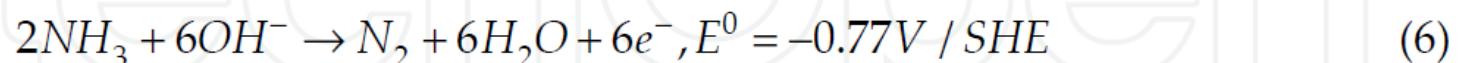
This reaction is endothermic. The temperature required for efficient cracking depends on the catalyst. There are a wide variety of materials that have been found to be effective, but some (e.g., supported Ni catalysts) require temperatures above 1000°C. Others have high conversion efficiency at temperatures in the range of 650-700°C. These temperatures are well above PEM fuel cell operating temperatures.

The viability of an ammonia-based on board storage system would depend largely on the following factors:

1. Development of high power, small volume, lightweight and efficient integrated ammonia cracking/purification systems capable of supplying hydrogen.
2. Development of lightweight tanks capable of sustaining the weight and vapor overpressure of anhydrous ammonia and with proven long-term integrity in an ammonia environment.
3. Addressing all of the safety issues associated with working with ammonia and ammonia containing systems.

2.3. Electrolysis of Ammonia

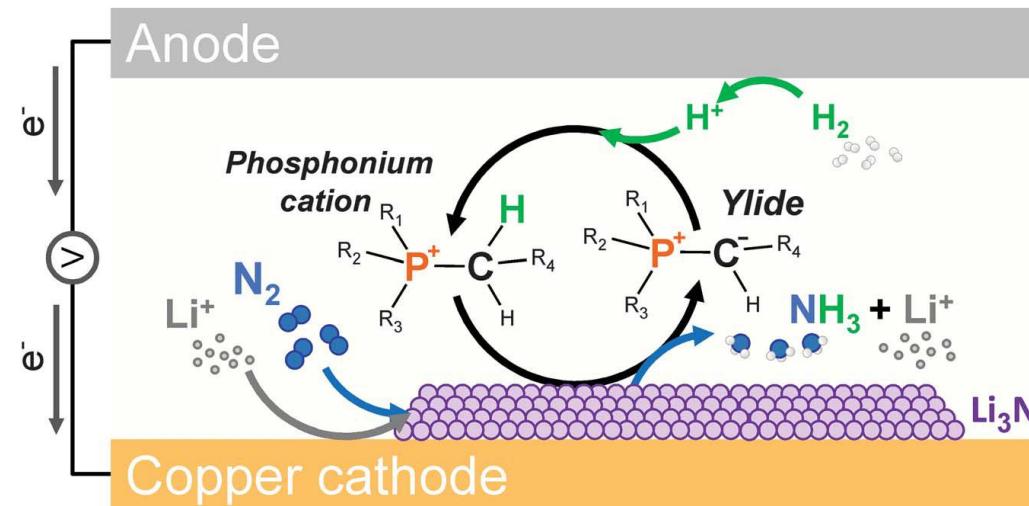
Electrolysis or electro-oxidation is another method of extracting hydrogen from ammonia. It has the advantage of scalability and versatility to interface with renewable energy sources including those whose electricity production varies with time [35]. Hydrogen can also be produced at moderate temperatures. It was first discussed by Vitse et al [35], who proposed the coupling of ammonia oxidation in an alkaline medium at the anode with the reduction of water at the cathode.



The thermodynamic potential for ammonia electrolysis in alkaline media is -0.77 V compared with -1.223 V for the electrolysis of water. The theoretical thermodynamic energy consumption is 1.55 Wh/g of H₂ from electrolysis of NH₃ compared to 33 Wh/g of H₂ from H₂O. This means that theoretically, ammonia electrolysis consumes 95% less energy to produce a quantity of hydrogen than water electrolysis

Green ammonia!

Nitrogen reduction to ammonia at high efficiency and rates based on a phosphonium proton shuttle: [Science 372, 1187–1191 \(2021\)](#)



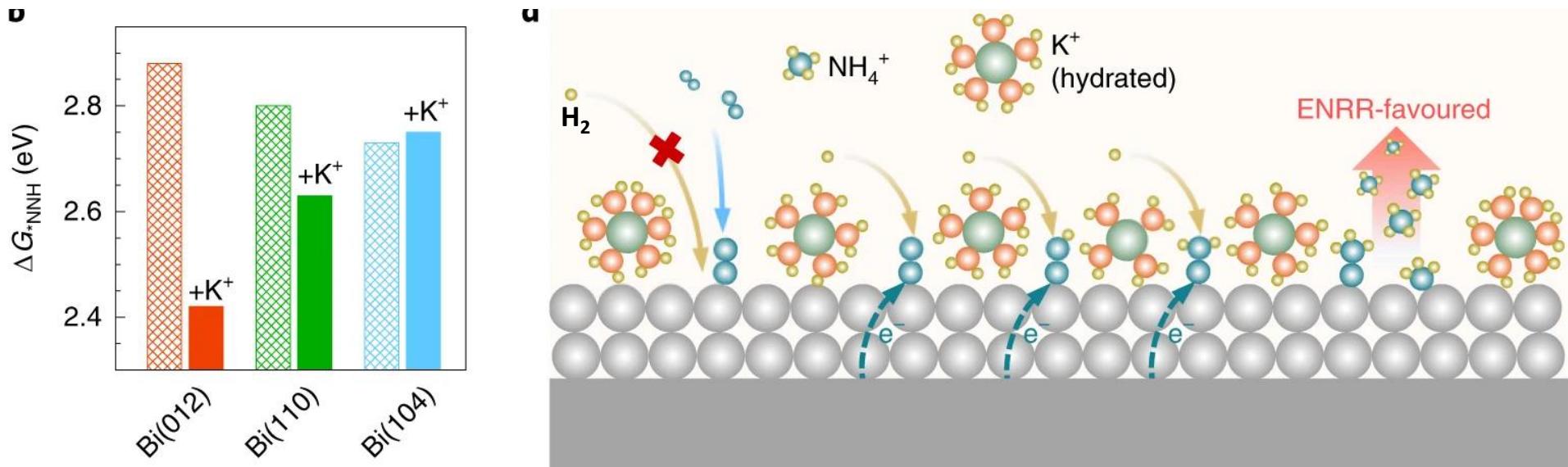
The cathode process involves the reduction of Li^+ to Li^0 which reacts with N_2 to produce Li_3N . This on protonation release NH_3 . The proton carrier is the phosphonium cation, which forms an ylide structure in its deprotonated state; this cycles to the anode where it is regenerated back to the phosphonium form through the reaction with H^+ derived from the oxidation of H_2 .

The salt also provides additional ionic conductivity, enabling high NH_3 production rates of 53 ± 1 nanomoles per second per square centimeter at $69 \pm 1\%$ faradaic efficiency in 20-hour experiments under 0.5-bar hydrogen and 19.5-bar nitrogen. Continuous operation for more than 3 days is demonstrated.

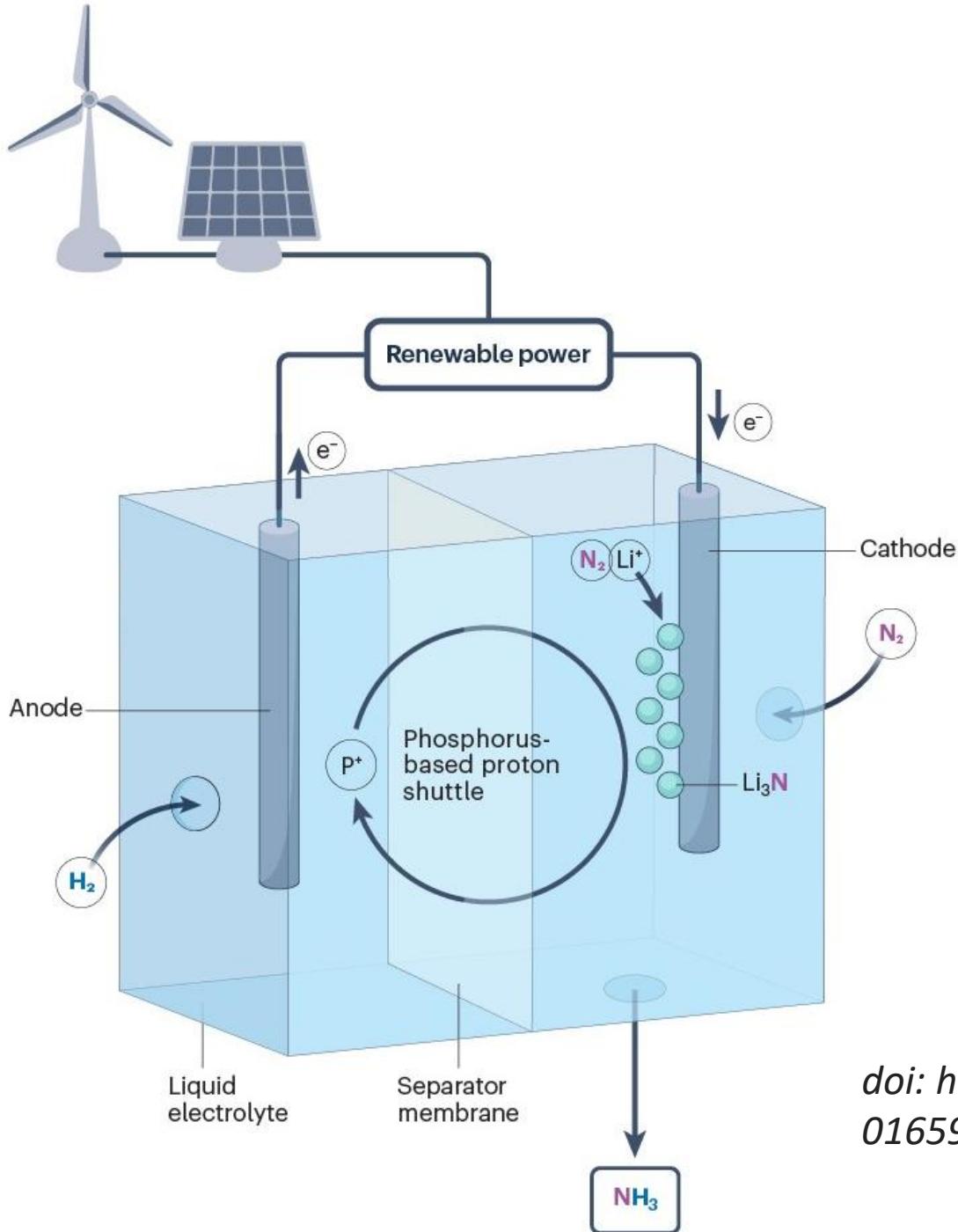
Promoting nitrogen electroreduction to ammonia with bismuth nanocrystals and potassium cations in water.

Nature Catalysis | VOL 2 | MAY 2019 | 448–456

A strategy to simultaneously promote ENRR (electrochemical nitrogen reduction reaction) selectivity and activity using bismuth nanocrystals and potassium cations. Bismuth exhibits higher intrinsic ENRR activity than transition metals due to the strong interaction between the Bi 6p band and the N 2p orbitals. This helps in lowering free-energy change (ΔG). Potassium cations stabilize key nitrogen-reduction intermediates and regulate proton transfer to increase selectivity. These further lower the ΔG . High Faradaic efficiency of 66% and ammonia yield of $200 \text{ mmol g}^{-1} \text{ h}^{-1}$ ($0.052 \text{ mmol cm}^{-2} \text{ h}^{-1}$) are obtained in the aqueous electrolyte under ambient conditions.



K^+ hinders proton transfer to the catalyst surfaces. Nitrogen will be adsorbed preferentially, and the ENRR is promoted

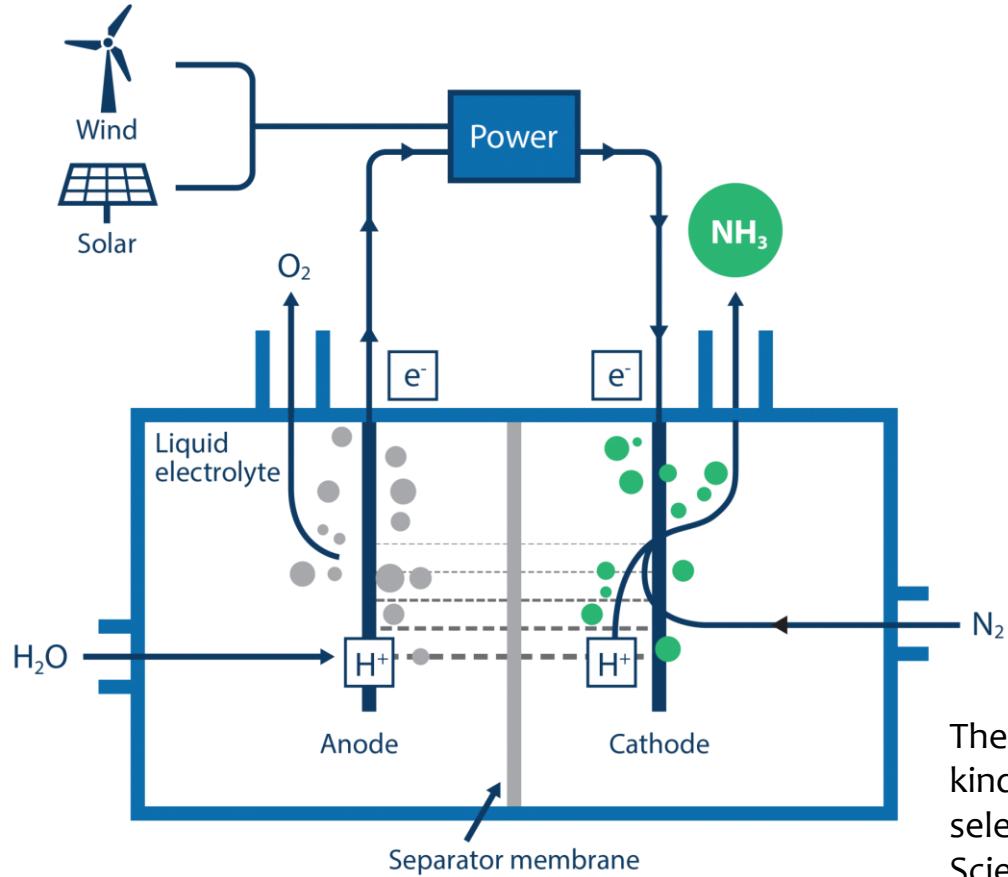


Jupiter Ionics in Melbourne, Australia, spun off from Monash University, Melbourne, in 2021.

It is a curious quirk of chemistry that when lithium atoms work together, they can break one of the strongest known chemical bonds. Lithium can take the triple-bonded nitrogen molecule (N_2) and, under ambient conditions, break it in two.

A report in Nature OUTLOOK
24 May 2023

doi: <https://doi.org/10.1038/d41586-023-01659-w>



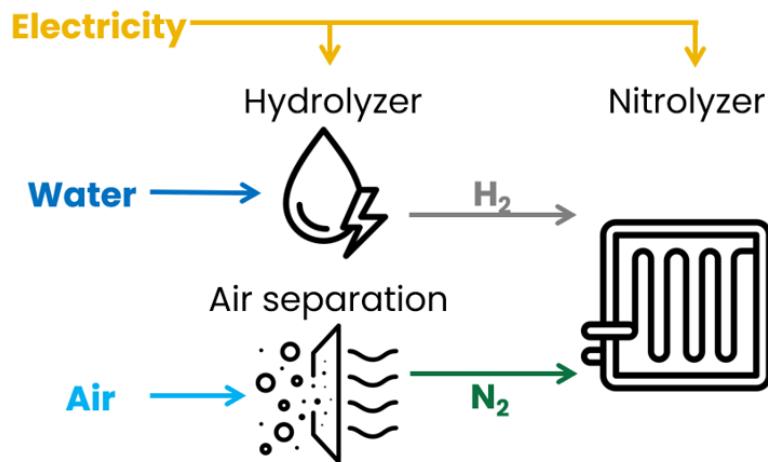
*A cell comprises two separated electrodes in a conductive liquid or gel electrolyte. Battery cells use chemical reactions to generate electrical energy. Conversely, electrolytic cells like ours use electrical energy to drive chemical reactions.

The MacFarlane Simonov Ammonia Cell is the first of its kind to demonstrate ammonia generation with 100% selectivity, and has shown good stability in lab tests. *Science*, 2021, 372, 1187-1191, 10.1126/science.abg2371



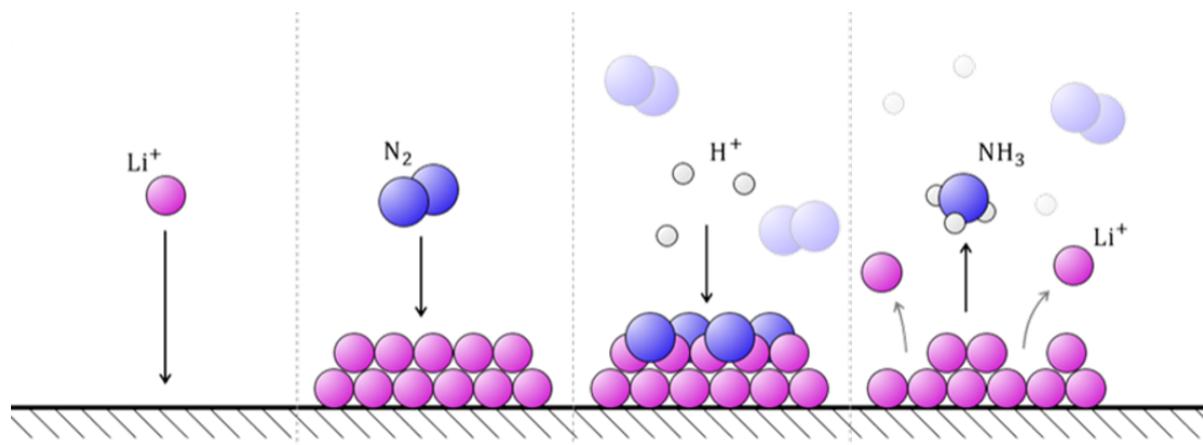
Our Technology

We use air, water, and renewable energy in a patented electrochemical process to produce green ammonia.



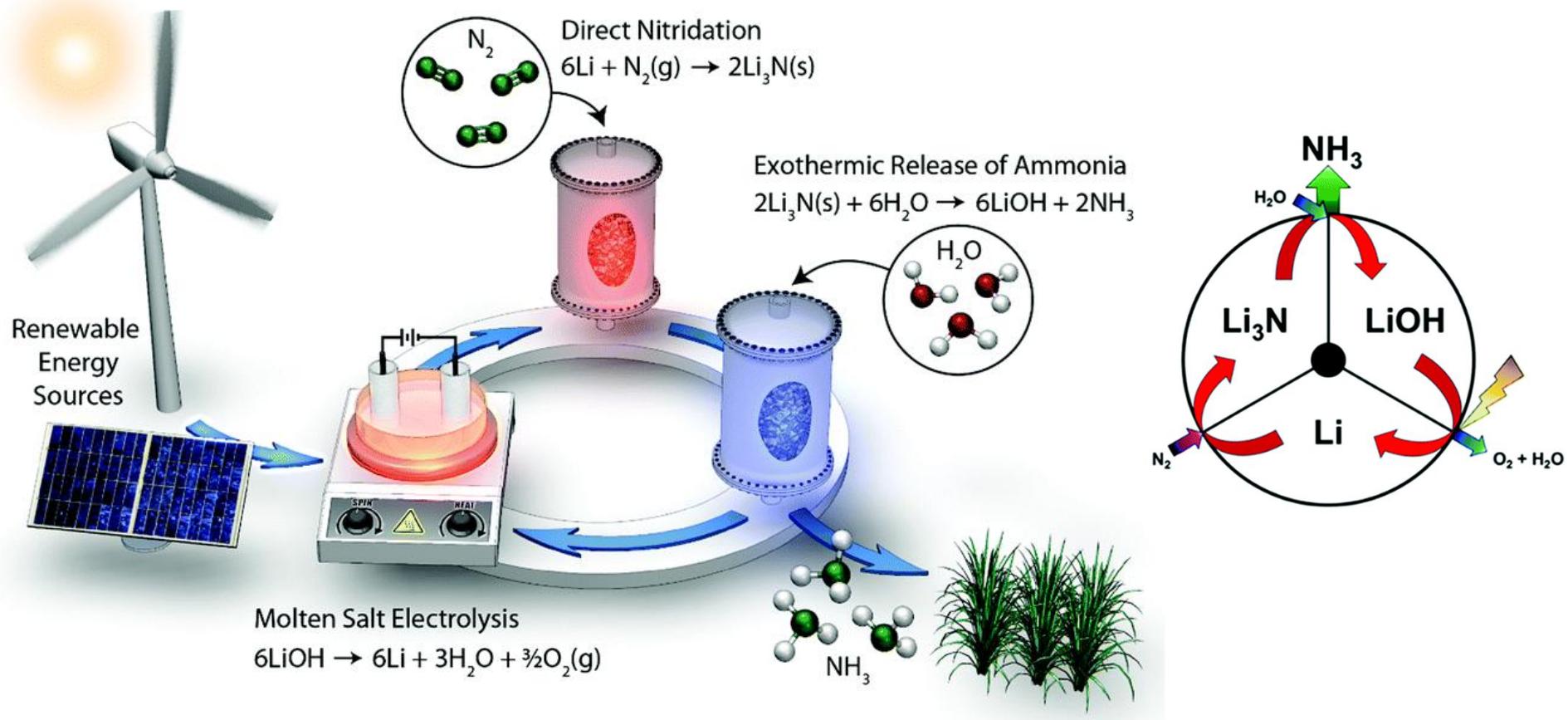
<https://www.nitrovolt.com/technology#solution>

<----- Room Temperature & Low Pressure ----->



The process happening inside the Nitrolyzer unit is based on the reduction of lithium salt to metallic lithium. This metallic lithium will then react with nitrogen to form a nitride. The nitride is easily protonated by hydrogen sourced via water splitting. This leads to the formation of ammonia, and the lithium is released back into solution, to be recycled and start the reaction again. This process happens continuously in our patent-pending flow-cell reactor, making ammonia on demand.

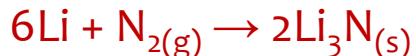
Ammonia synthesis from N₂ and H₂O using a lithium cycling electrification strategy at atmospheric pressure



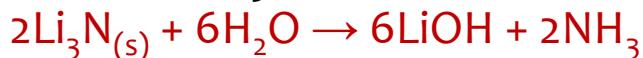
Step 1: LiOH electrolysis: Total cell: $6\text{LiOH} \rightarrow 6\text{Li} + 3\text{H}_2\text{O} + 3/2\text{O}_{2(g)}$

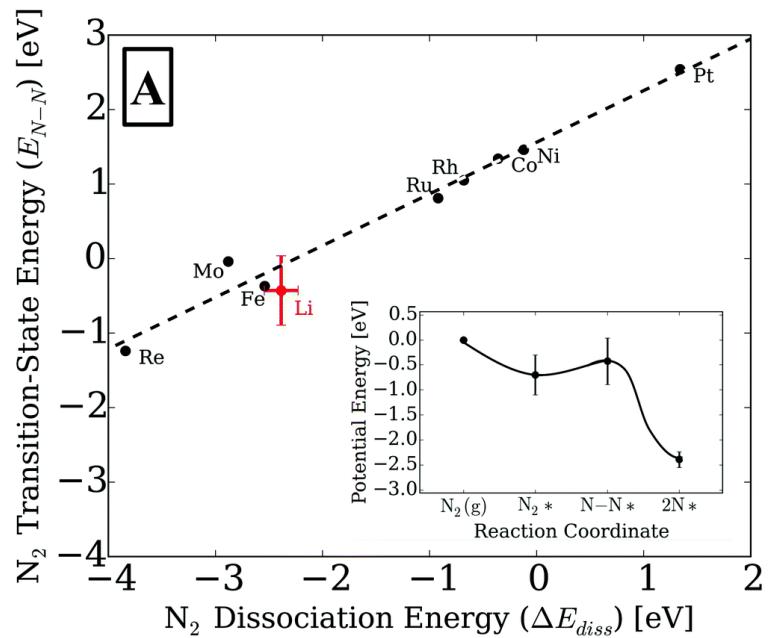


Step 2: Direct reaction of metallic Li with N₂ to form Li₃N



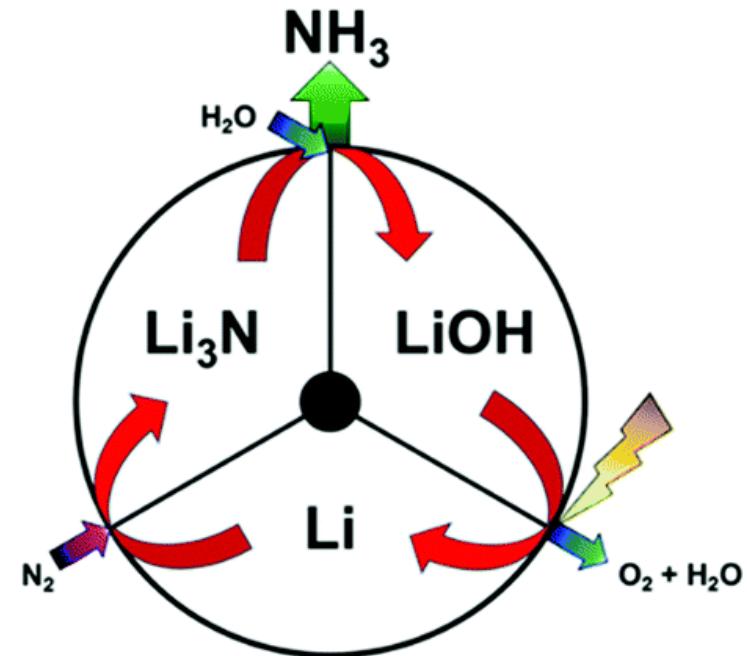
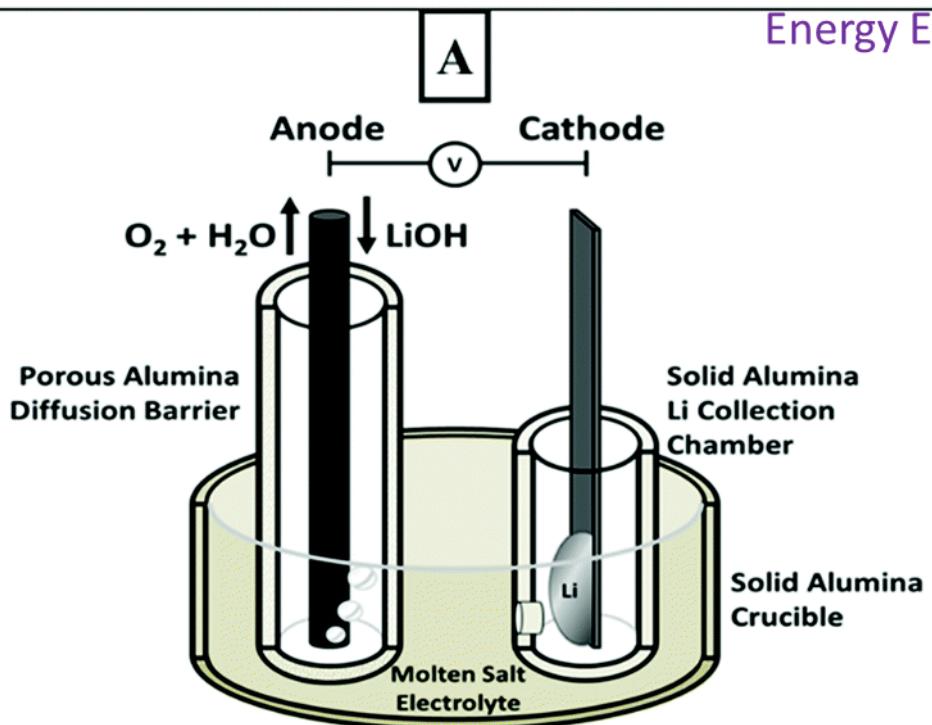
Step 3: Release of NH_3 by reaction with H_2O :





The three steps of the demonstrated process are LiOH electrolysis, direct nitridation of Li, and the exothermic release of ammonia from Li_3N , which reproduces the LiOH, completing the cycle. The process uses N_2 and H_2O at atmospheric pressure and reasonable temperatures, and, while approaching industrial-level electrolytic current densities, we report an initial current efficiency of 88.5% toward ammonia production

Energy Environ. Sci., 2017, 10, 1621-1630



Membrane electrode assembly: The sequential parts of membrane electrode assembly (MEA) are anode diffusion layer (ADL), anode catalyst layer (ACL), electrolyte membrane, cathode catalyst layer (CCL) and cathode diffusion layer (CDL). Both the electrodes are supported on macroporous carbon paper or carbon cloth called as diffusion layer backing.

Electrolyte membrane: The most common and important part in the MEA is the electrolyte membrane which separates the anode and the cathode compartment and also acts as a proton carrier. Perfluorinated polymer membrane, known as Nafion®, is the most commonly used membrane in the passive DMFC due to their high chemical stability, mechanical strength, thermal stability and excellent proton conductivity (0.1 S cm^{-1} in the fully hydrate state).

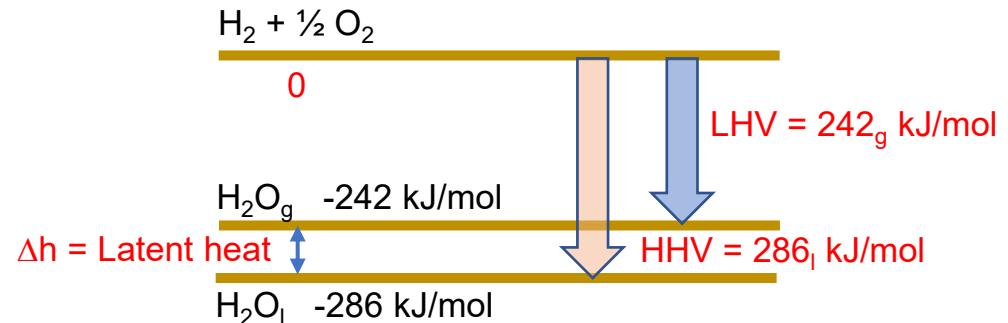
Requirements of electrolyte membrane The common requirements of passive DMFCs membranes to expand the passive DMFC commercialization are & Low methanol crossover (MCO) & High ionic conductivity & High mechanical and chemical durability & High stability and strength of membrane & High operation temperature & Low cost & Low Ru crossover (if anode catalyst contains Ru)

Requirements of anode catalyst Anode electrode serves two purposes; it effectively collects electrons and also delivers/ collects reactants (MeOH) and product (CO_2) species. Thus, anode electrode must also provide: & High catalytic activity & High porosity & High electrical conductivity & High surface area & Highly stable and durable & Low cost & Significantly lower affinity to CO.

Efficiency loss in the Fuel Cell

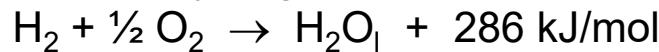
High Heating value (HHV) of H₂ combustion (H₂ + excess O₂) is measured in calorimetric bomb Product: Water [H₂O_l @ 25°C]

Low Heating value (LHV) of H₂ combustion (H₂ + excess O₂) is measured in calorimetric bomb Product: Vapour [H₂O_g]

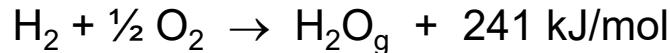


At 25°C

HHV of Hydrogen



LHV of Hydrogen



$$HHV - LHV = \text{latent heat } (\Delta h) = 45 \text{ kJ/mol}$$

$$HHV = LHV + \Delta h \times (n_{H_2O[OUT]} / n_{fuel[in]})$$

These observations indicate that the equilibrium potential of a fuel cell is determined by the equilibrium between the chemisorbed gases and the electrolyte, rather than between the free gases and the electrolyte. Since chemisorption is not reversible for this purpose—the heat of chemisorption is dissipated before reaction occurs—a higher heat of chemisorption causes a greater deviation of the cell potential from its theoretical value. Experimental results show that the open-circuit potential varies with the heat of chemisorption of hydrogen on the catalyst, demonstrating that the equilibrium involves chemisorbed hydrogen. Consequently, the electrode catalyst plays a dual role: it not only governs the open-circuit potential but also enhances the kinetics of the electrochemical reactions.



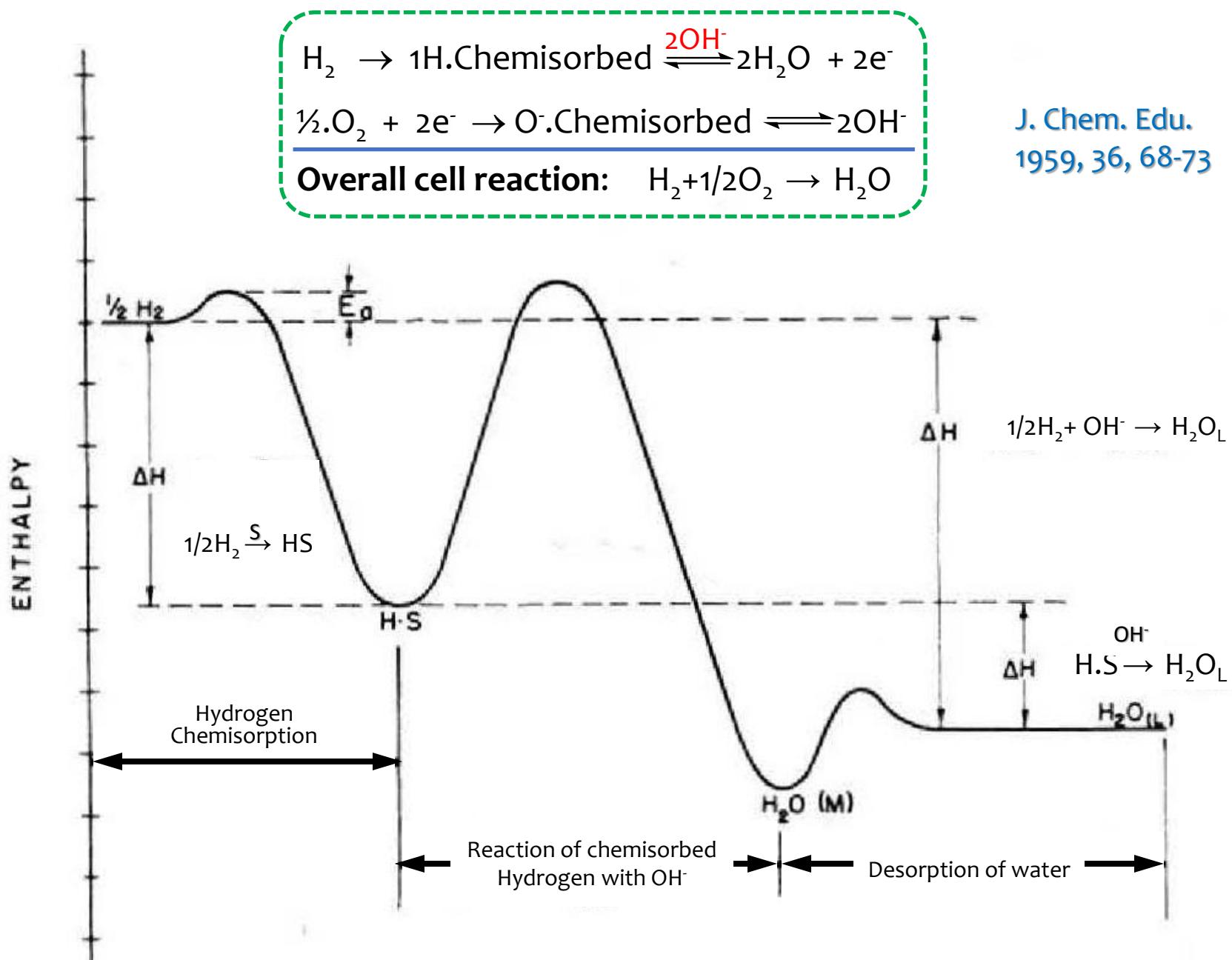
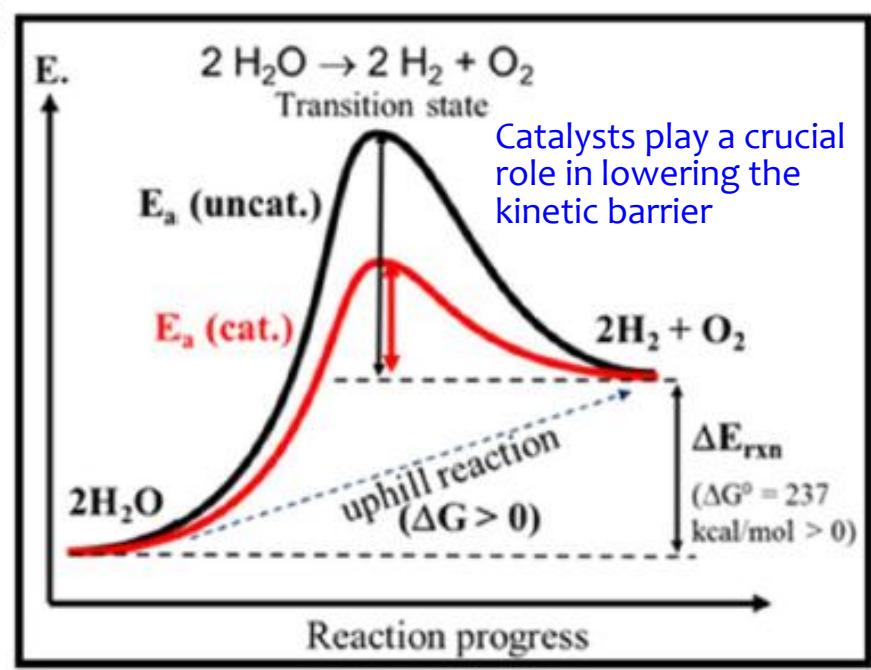
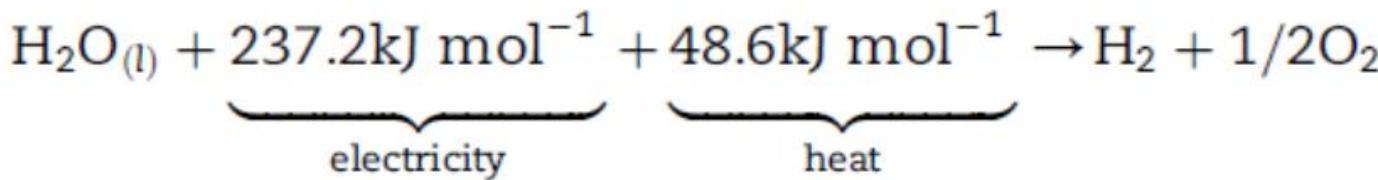


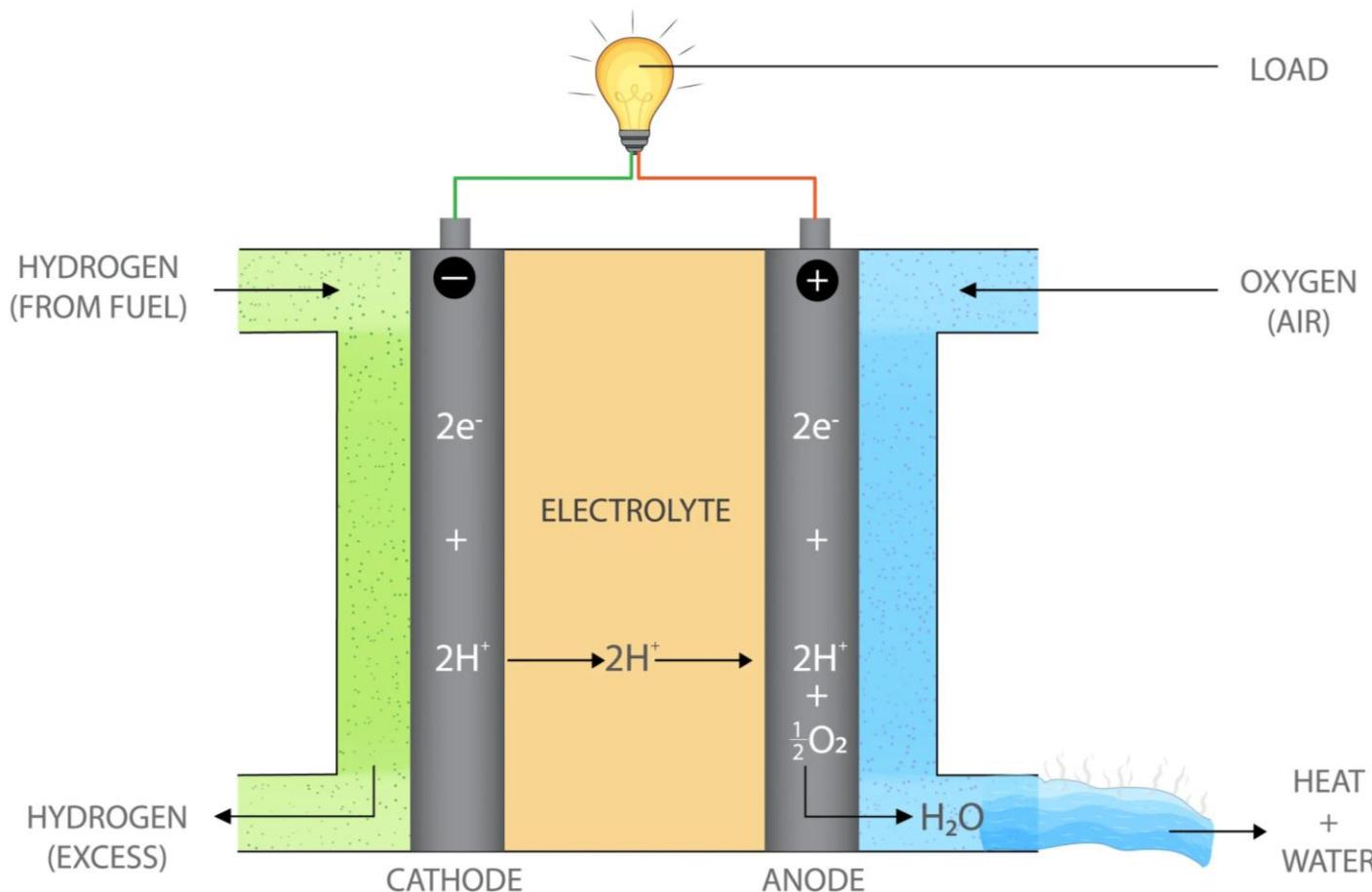
Figure 6. Course of the reaction at the hydrogen electrode.



Yttria (Y_2O_3) is added to zirconia to create yttria-stabilized zirconia (YSZ) — a stable, oxygen-ion-conducting ceramic that is crucial for the electrolyte and anode support in SOFCs.

- Platinum (Pt).
 - Alloy catalysts such as Pt–Ru, Pt–Ni, and Pt–Co improve CO tolerance
 - Non-precious catalysts, including transition-metal oxides (e.g., MnO_2 , Co_3O_4 , Fe–N–C complexes), nitrogen-doped carbon materials, and conductive polymers
 - In solid oxide fuel cells (SOFCs), high-temperature operation allows the use of non-noble catalysts such as Ni-based cermets at the anode and perovskite-type oxides (e.g., $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$) at the cathode

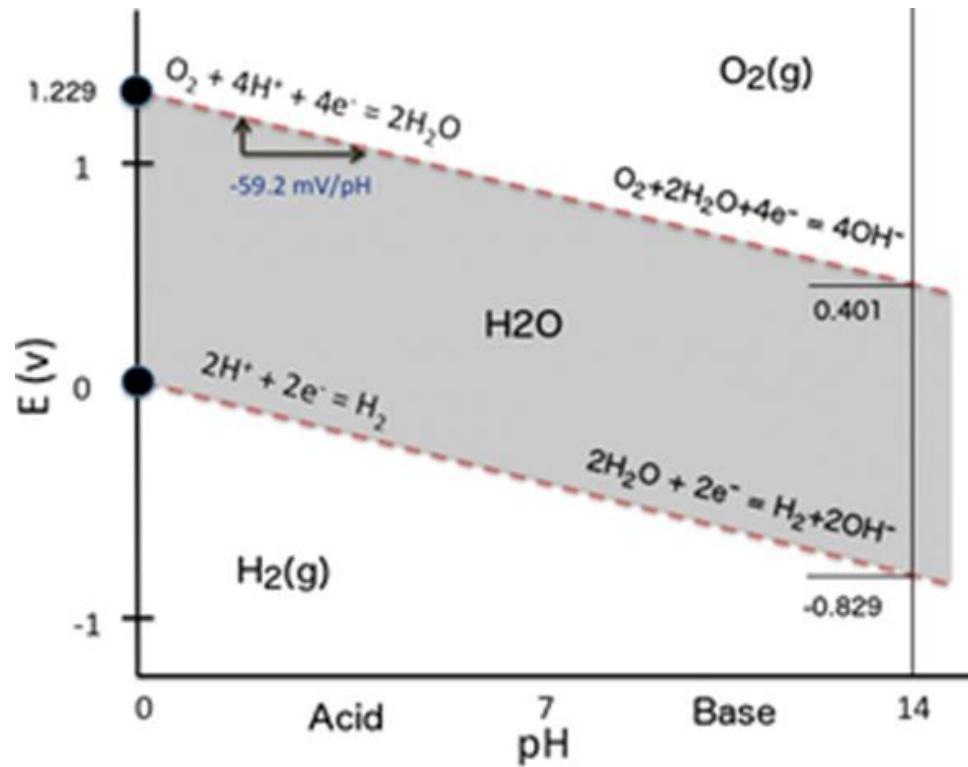
A fuel cell is an electrochemical device that continuously converts the chemical energy of a fuel (typically hydrogen) and an oxidant (usually oxygen or air) into electrical energy, accompanied by heat and reaction products such as water. Unlike a battery, which operates using stored reactants in a closed system, a fuel cell requires a continuous external supply of fuel and oxidant to sustain its operation.



Fuel cells are electrochemical devices to convert chemical energy into electrical energy. They offer higher electrical efficiency ($\geq 40\%$) compared to conventional power generation systems such as reciprocating engine ($\approx 35\%$), turbine generator (30–40) %, photovoltaics (6–24) % and wind turbines ($\approx 25\%$). Other advantages include fuel flexibility, base load and off-grid applications. Noise-free operation and modular construction are added features that allow its further application in small residential, automotive, portable electronic devices, as well as off-grid electricity generation in remote areas, marine and space applications.

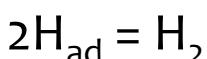
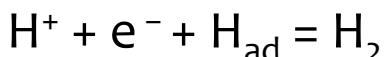
H_2 has the highest gravimetric energy density. When it is used as the fuel in a fuel cell, it features not only high efficiency in energy conversion, but also produces zero pollution as it emits only water as a byproduct. **Efforts on water splitting cells for H_2 production from renewable sources and fuel cells for effective conversion of H_2 to electricity has become a global drive towards a sustainable power package of the future.**

The thermodynamic potential is 1.23 V at 25 °C and 1 atm. However, due to the kinetic barrier for the reaction, water electrolysis requires a higher potential than thermodynamic potential (1.23 V) to overcome the kinetic barrier. The excess potential is also known as overpotential (η) which mainly comes from the intrinsic activation barriers present on both anode and cathode.

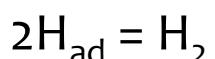
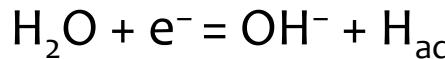


Overpotential serves as a quantitative descriptor of catalytic performance:
 Low overpotential → high catalytic activity and efficiency
 High overpotential → sluggish kinetics and poor catalytic performance

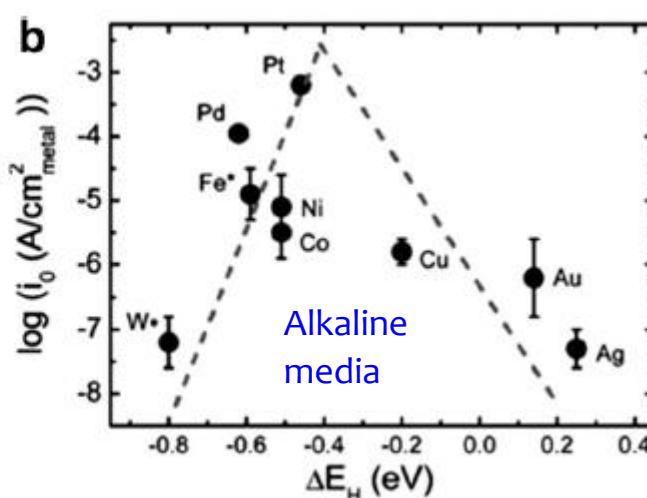
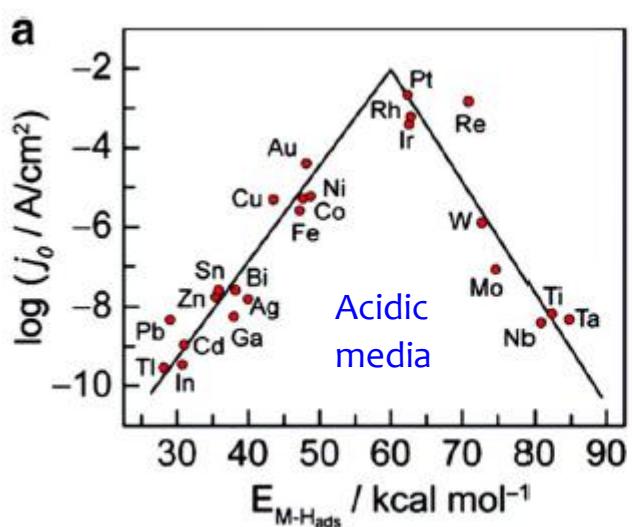
H_2 evolution Reaction in pH < 7



H_2 evolution Reaction in pH > 7



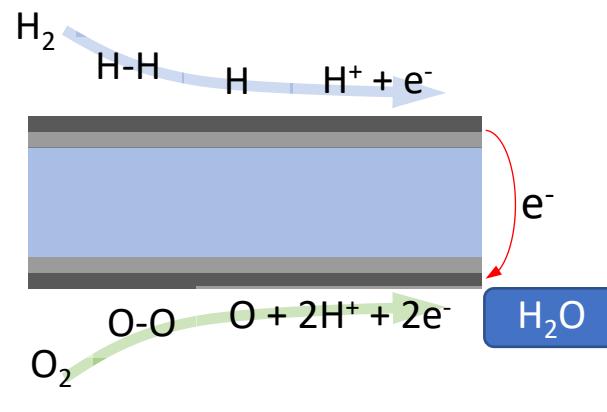
It is vital to trade off H_{ad} , hydroxy adsorption (OH_{ad}), and water dissociation from the catalytic surface for HER activity in alkaline media. The free energy of hydrogen adsorption (ΔG_H) is widely accepted to be a descriptor for a hydrogen evolution material. A moderate value of hydrogen binding energy will benefit HER process.



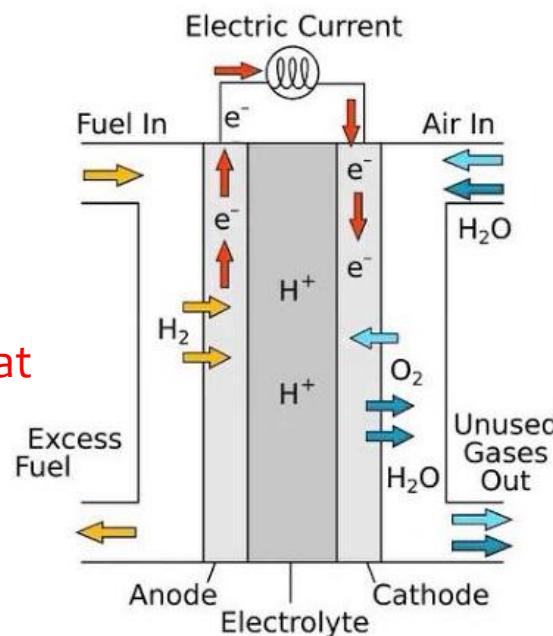
Volcano plots: a exchange current density vs. the M–H bond energy for each metal surface; b exchange current density on monometallic surfaces vs. the calculated HBE (for alkaline media)

A fuel cell is an electrochemical cell that converts the chemical energy of a fuel (often hydrogen) and an oxidizing agent (often oxygen) into electricity through a pair of redox reactions.

Fuel cells are different from most batteries in requiring a **continuous source of fuel and oxygen (usually from air) to sustain the chemical reaction**, whereas in a battery the chemical energy usually comes from metals and their ions or oxides that are commonly already present in the battery, except in flow batteries. Fuel cells can produce electricity continuously for as long as fuel and oxygen are supplied.

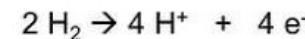


Overall Reaction



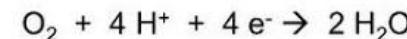
Fuel Cell

AT THE ANODE (- electrode)
OXIDATION TAKES PLACE

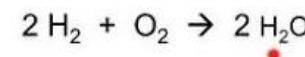


These H^+ ions move through the electrolyte (often a polymer or membrane)

AT THE CATHODE (+ electrode)
REDUCTION TAKES PLACE



OVERALL REACTION



Selective Proton Transport in Fuel Cell Electrolytes:

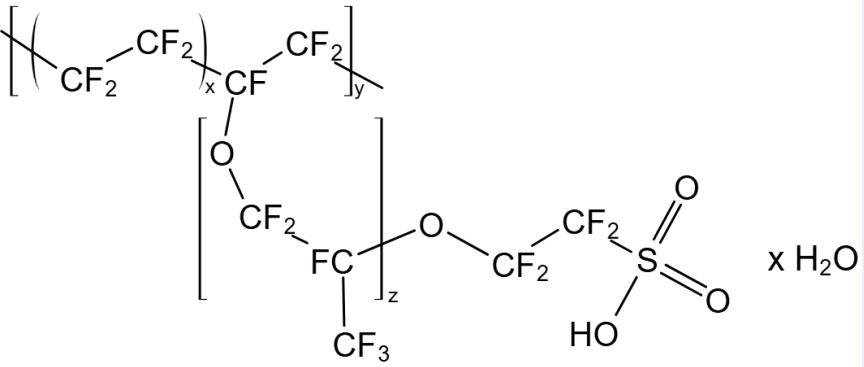
In a proton-exchange membrane fuel cell (PEMFC), the electrolyte (membrane) is specifically designed to conduct protons (H^+) while blocking electrons and gases such as H_2 and O_2 . This selective ion transport is essential to maintain charge balance and electrical isolation between the electrodes.

1. Structure of the Electrolyte

The most common electrolyte is Nafion, a **perfluorosulfonic acid (PFSA)** polymer consisting of:

- A hydrophobic fluorocarbon backbone (like Teflon) for mechanical and chemical stability.
- Hydrophilic sulfonic acid ($-SO_3H$) side groups that attract and hold water.

When hydrated, the sulfonic acid groups dissociate, forming mobile protons (H^+) and negatively charged $-SO_3^-$ sites that are fixed to the polymer framework.



Nafion is currently a brand of
the Chemours company

Mechanism of Proton Conduction

H^+ move through the membrane via two primary mechanisms:

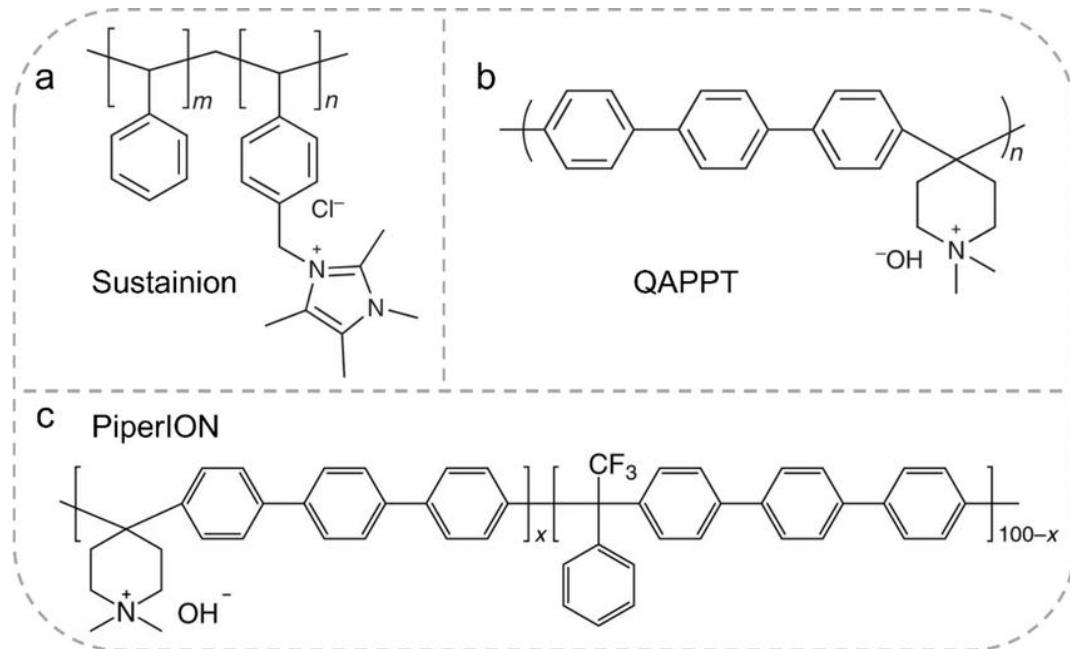
- **Vehicle mechanism:** Protons associate with H_2O molecules to form hydronium ions (H_3O^+), which diffuse through interconnected water channels.
$$H_3O^+ \rightarrow H_2O + H^+$$
- **Grotthuss (hopping) mechanism:** Protons "hop" along a network of H-bonds between H_2O molecules and SO_3H^- groups, rapidly transferring charge without significant mass transport.

Alkaline polymer electrolytes (anion exchange membranes, AEMs) are being developed to replace liquid KOH.

Examples: quaternary ammonium-functionalized polymers (e.g., FAA-3, Sustainion®, PiperION™).

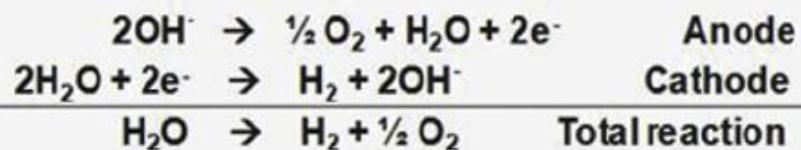
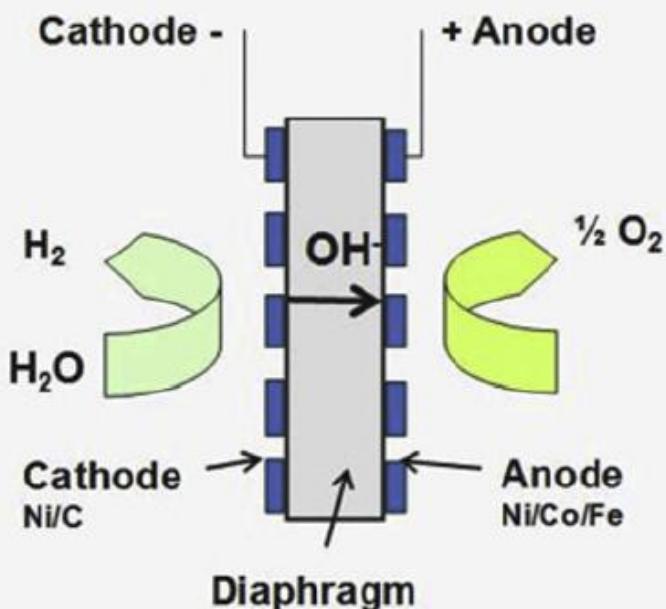
Advantages: reduced CO₂ sensitivity, no electrolyte leakage, improved durability.

In short, **aqueous KOH** is the traditional electrolyte for AFCs, while **solid AEMs** represent the next generation for safer and more efficient alkaline fuel cells.



Alkaline electrolysis

40 - 90 °C



PEM electrolysis

20 - 100 °C

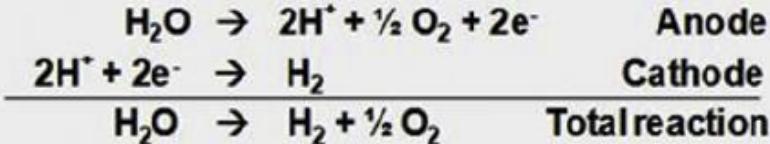
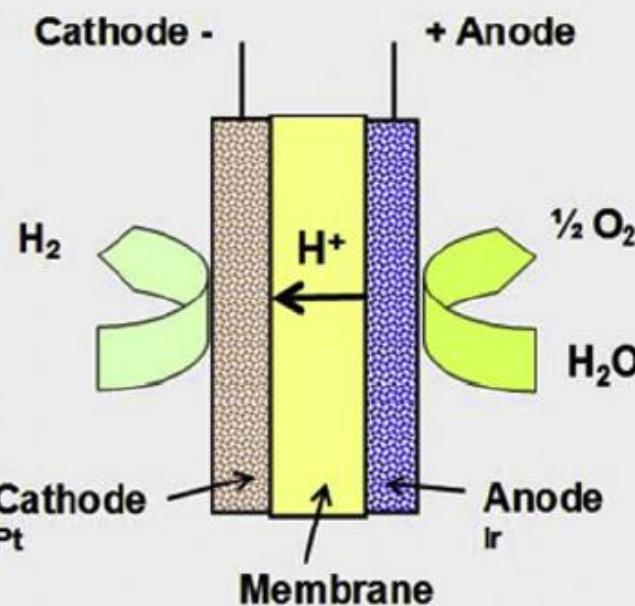
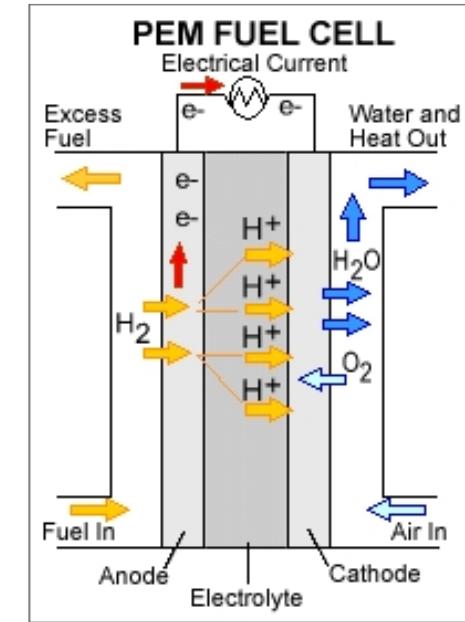
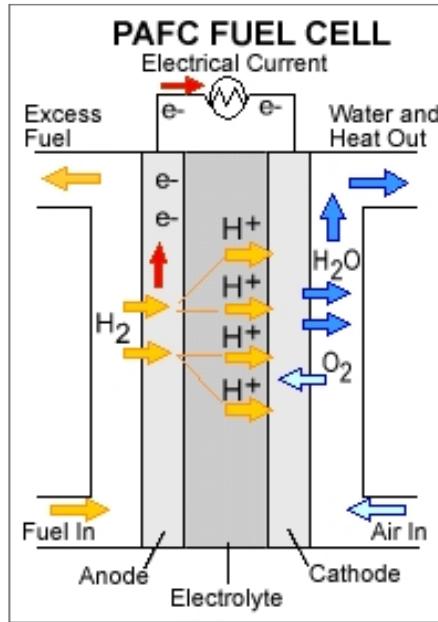
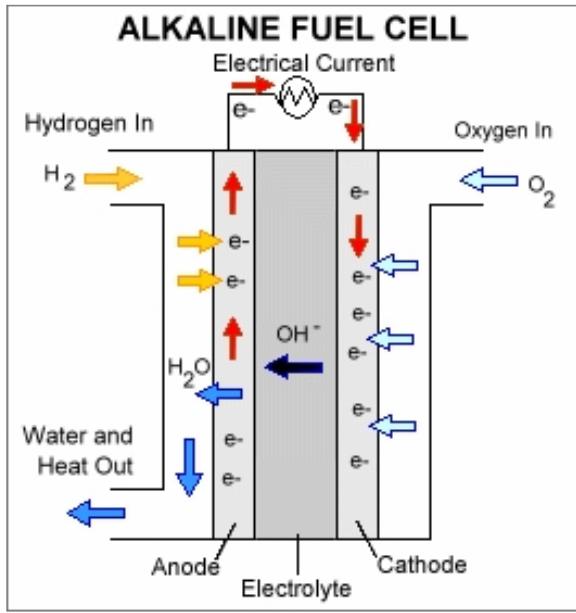


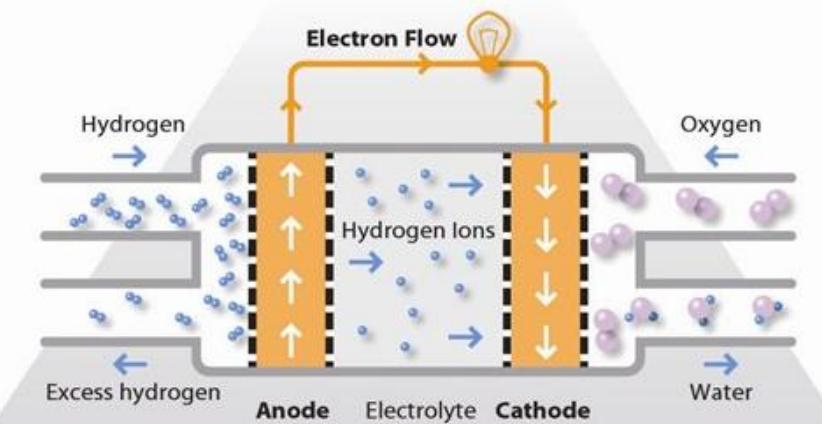
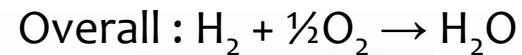
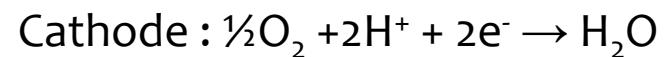
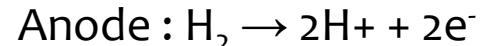
Fig. 2 – Schematic of the operating principle of an alkaline and PEM water electrolysis cell.



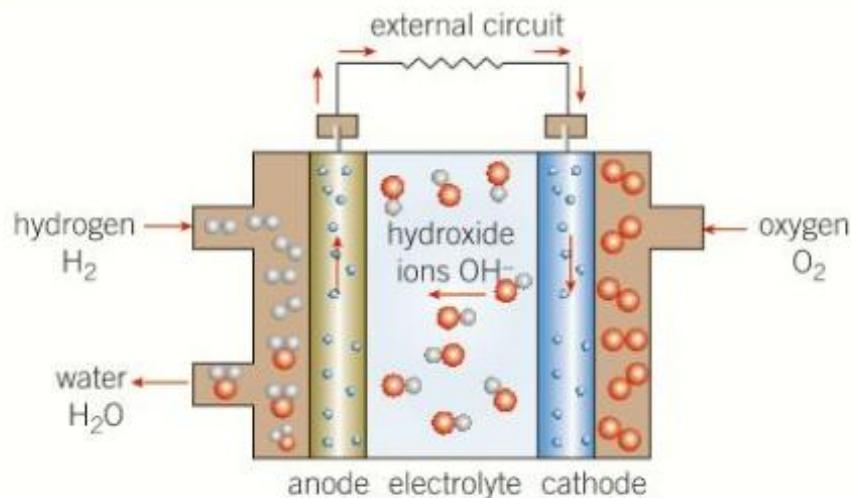
Phosphoric acid fuel cells (PAFC): Introduced for the first in early 1960s. Acid electrolyte cells are more tolerant to CO_2 and allow the use of normal air and nonpure hydrogen.

Proton exchange membrane (PEM) fuel cells also called polymer electrolyte membrane fuel cells (**PEMFC**) use a water-based, acidic polymer membrane as the electrolyte with Pt-based electrodes. Limited by its stability, it works at a relatively lower temperature ($< 100^\circ C$). Polymer which selectively allows protons to be diffused from one face to the other (fluoropolymer (PFSA) Nafion, a DuPont product.

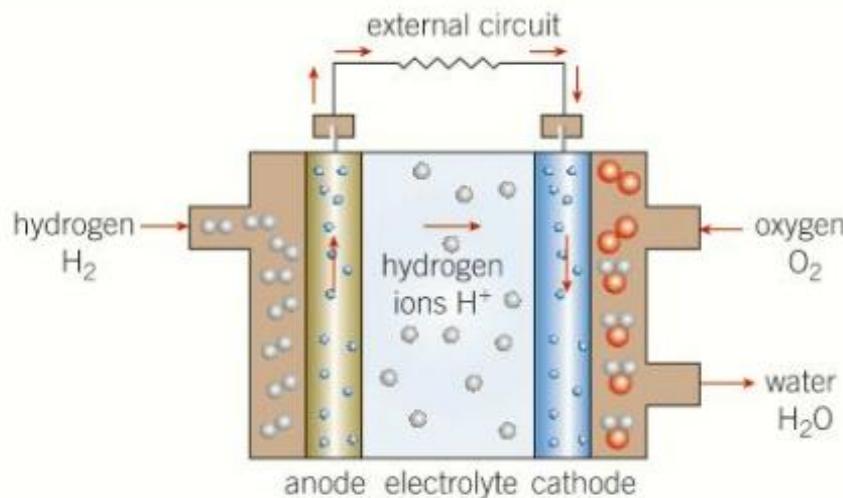
PEMFC



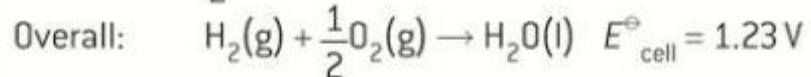
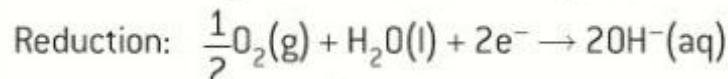
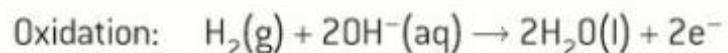
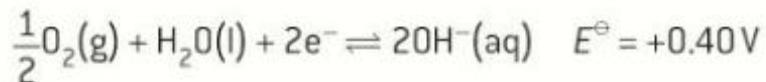
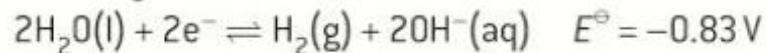
Alkali hydrogen fuel cell



Acid hydrogen fuel cell



Redox systems



Redox systems

