University of Nottingham
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Materials in Design
MMME2045

Block F: Designing with Functional Materials

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BLOCK 4: Designing with Functional Materials

In this Block we will cover

1. **Energy materials**

Case study: energy materials and systems (fuel cells, lithium ion batteries, lead acid batteries, supercapacitors) for electric propulsion systems

2. **Ferromagnetic materials**

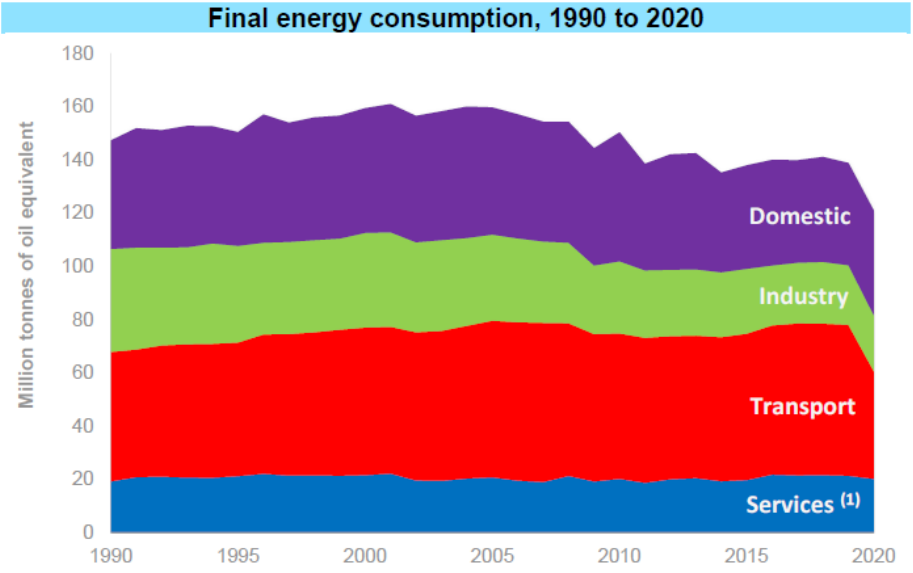
Case study: permanent magnets for motors and generators

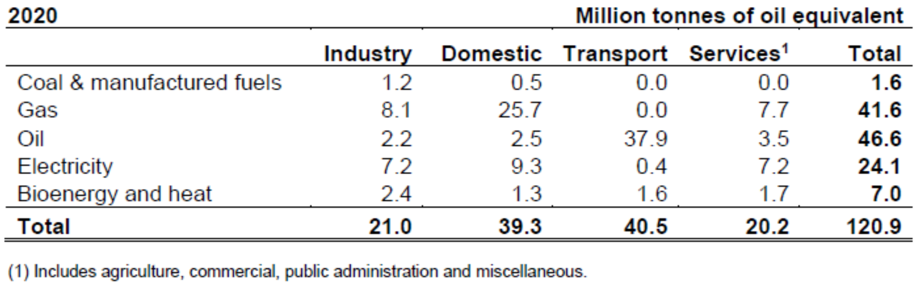
3. **Piezoelectric materials**

UK 2050 target:

To bring all greenhouse gas emissions to net zero by 2050.

OVERALL ENERGY



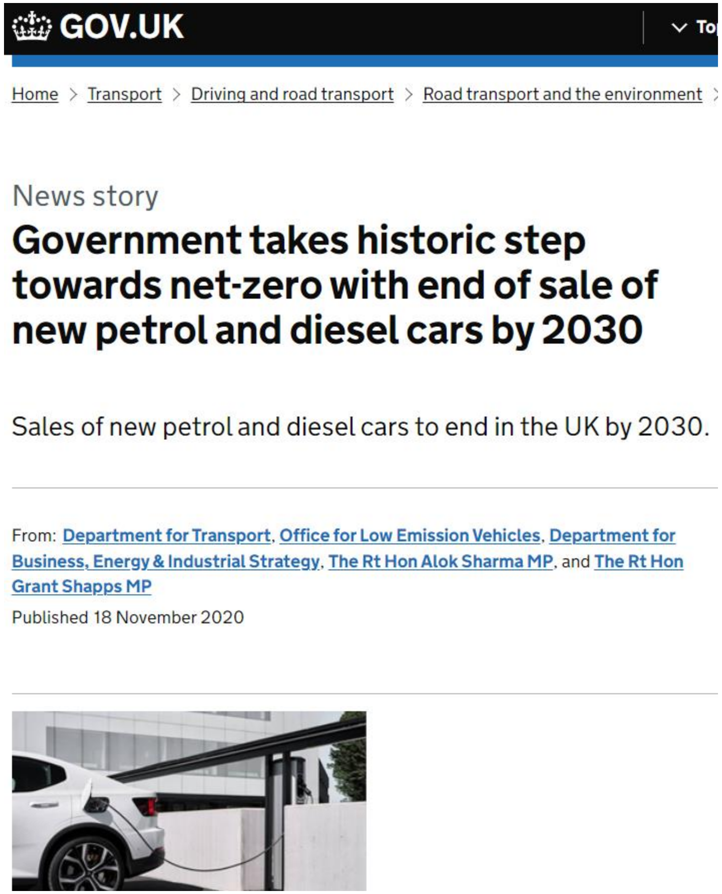


2020 — Million tonnes of oil equivalent

	Industry	Domestic	Transport	Services[1]	Total
Coal & manufactured fuels	1.2	0.5	0.0	0.0	**1.6**
Gas	8.1	25.7	0.0	7.7	**41.6**
Oil	2.2	2.5	37.9	3.5	**46.6**
Electricity	7.2	9.3	0.4	7.2	**24.1**
Bioenergy and heat	2.4	1.3	1.6	1.7	**7.0**
Total	**21.0**	**39.3**	**40.5**	**20.2**	**120.9**

(1) Includes agriculture, commercial, public administration and miscellaneous.

UK Energy in Brief 2021, Department for Business, Energy & Industrial Strategy (BEIS)



Home > Transport > Driving and road transport > Road transport and the environment >

News story

Government takes historic step towards net-zero with end of sale of new petrol and diesel cars by 2030

Sales of new petrol and diesel cars to end in the UK by 2030.

From: Department for Transport, Office for Low Emission Vehicles, Department for Business, Energy & Industrial Strategy, The Rt Hon Alok Sharma MP, and The Rt Hon Grant Shapps MP

Published 18 November 2020

Electric propulsion systems

Business

Economy | Companies | Opinion | Open economy | Markets | Alex | Telegraph Conn

Business

Rolls-Royce: the future of flight is electric

GE reveals major achievements in hybrid electric propulsion

25 AUGUST, 2017 | SOURCE: FLIGHTGLOBAL.COM | BY: STEPHEN TRIMBLE | WASHINGTON DC

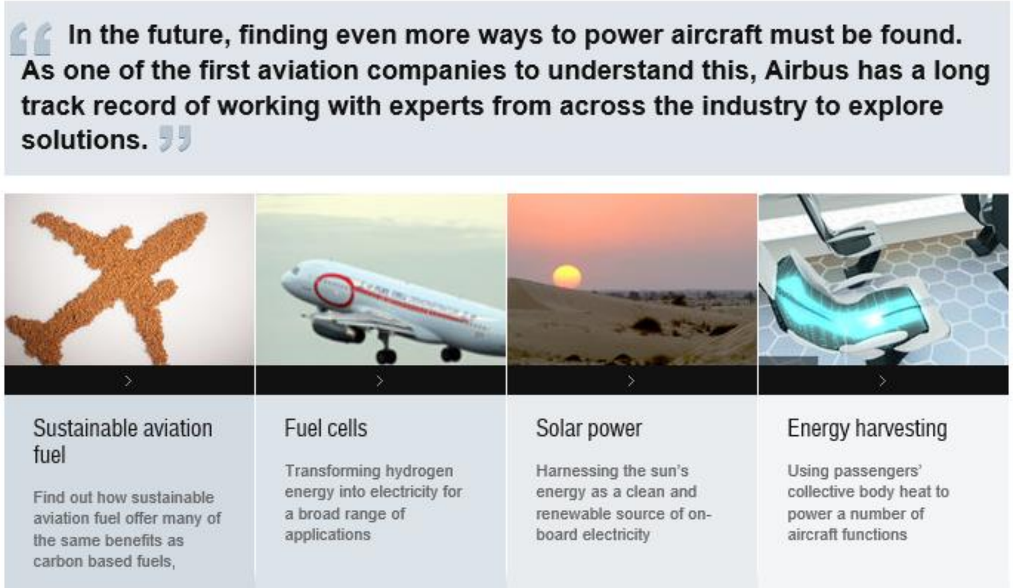
GE Aviation has broken a two-year silence on a major research project in hybrid electric propulsion with a new white paper that discloses several major advances demonstrated in two experiments since 2015 and that confirms the company is in talks with several potential aircraft makers about using the new technology.

Airbus and Siemens investigate hybrid-electric propulsion systems for low emission aviation

By **Helen Knight** 18th April 2016 8:34 am

Hybrid-electric aircraft that produce significantly lower emissions than existing aeroplanes could be in the sky by 2030, as a result of a collaboration between Airbus and Siemens.

AIRBUS



“In the future, finding even more ways to power aircraft must be found. As one of the first aviation companies to understand this, Airbus has a long track record of working with experts from across the industry to explore solutions.”

Sustainable aviation fuel

Find out how sustainable aviation fuel offer many of the same benefits as carbon based fuels,

Fuel cells

Transforming hydrogen energy into electricity for a broad range of applications

Solar power

Harnessing the sun's energy as a clean and renewable source of on-board electricity

Energy harvesting

Using passengers' collective body heat to power a number of aircraft functions

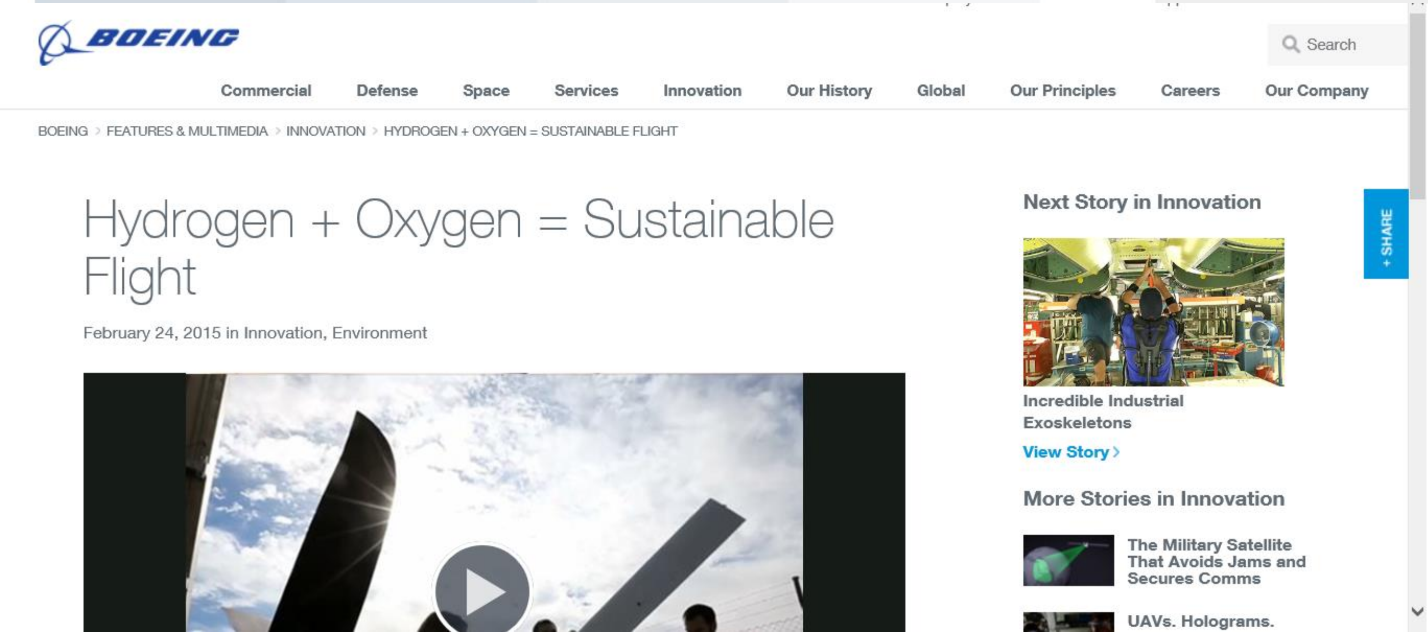
... / Future by Airbus / Future energy sources / Fuel cells

FUEL CELLS

Sustainable aviation fuel

ELECTRICITY THROUGH “COLD” COMBUSTION

Airbus and its partners are exploring the use of fuel cells to power aircraft systems.



BOEING > FEATURES & MULTIMEDIA > INNOVATION > HYDROGEN + OXYGEN = SUSTAINABLE FLIGHT

Hydrogen + Oxygen = Sustainable Flight

February 24, 2015 in Innovation, Environment

Next Story in Innovation

Incredible Industrial Exoskeletons

View Story >

More Stories in Innovation

The Military Satellite That Avoids Jams and Secures Comms

UAVs. Holograms.

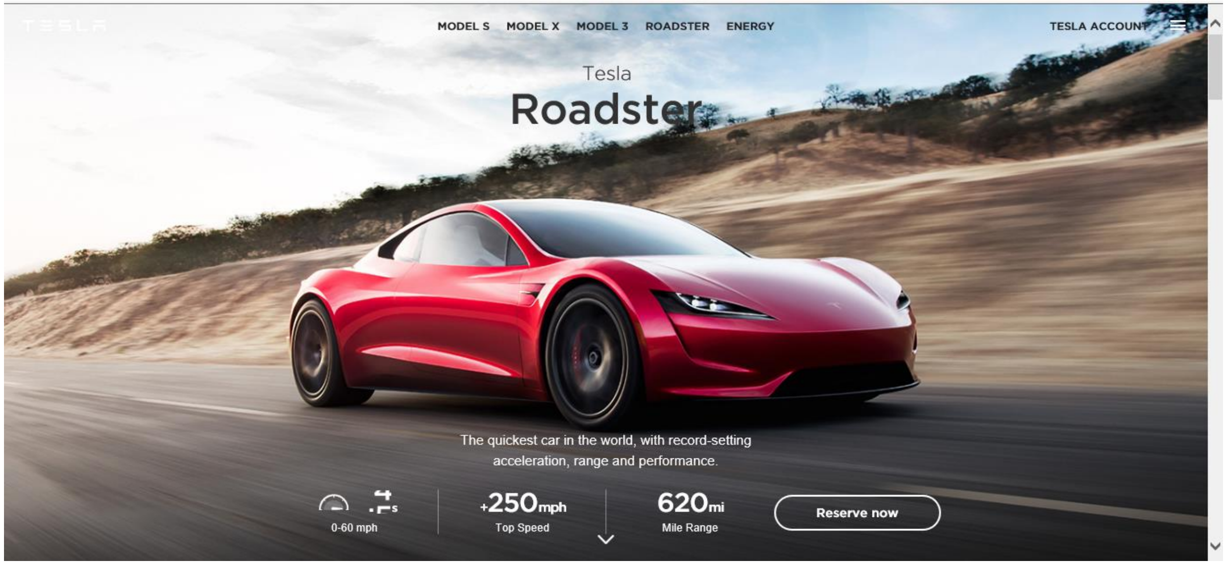
Tesla Roadster

0-60 mph: **1.9 s**

Range: **620 miles**

Top speed: **+250 mph**

Price: **£189,000**



Tesla
Roadster

The quickest car in the world, with record-setting acceleration, range and performance.

Tesla Model S

All cars have adaptive air suspension, premium interior and sound.

Dual Motor All-Wheel Drive

Long Range Plus	£79,980
Performance	£94,980

Tri Motor All-Wheel Drive

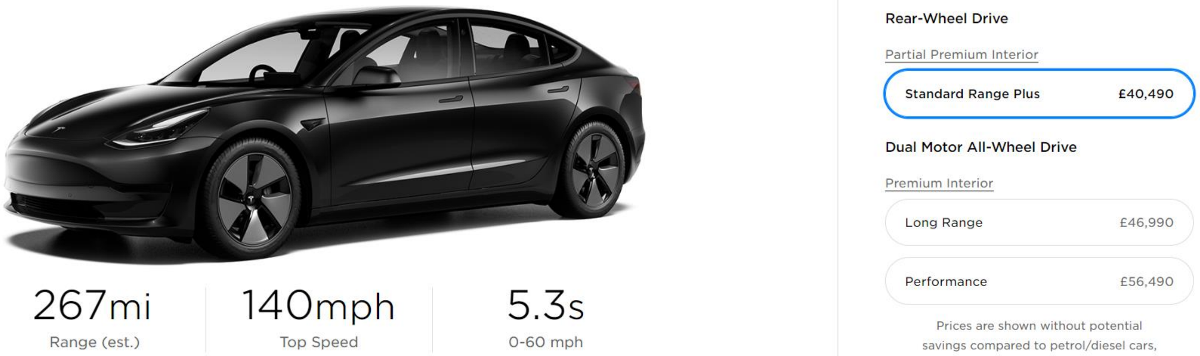
Plaid	£130,980

The only thing beyond Ludicrous mode is Plaid

Model S Performance includes:

- Quicker acceleration: 0-60 mph in 2.3s

Tesla Model 3



Rear-Wheel Drive

Partial Premium Interior

Standard Range Plus	£40,490

Dual Motor All-Wheel Drive

Premium Interior

Long Range	£46,990
Performance	£56,490

Prices are shown without potential savings compared to petrol/diesel cars,

Switching to electric vehicles


Nissan Leaf


BMW i3


Volkswagen ID.3


Audi e-tron i3


Mini Electric


Jaguar I-PACE

Hydrogen fuel cell cars and buses

Hyundai ix35

Toyota Mirai

Honda Clarity

AIR LIQUIDE Creative Oxygen, ALSTOM, AngloAmerican, BMW GROUP, DAIMLER, ENGIE by people for people

HONDA, HYUNDAI, Kawasaki, Shell, THE LINDE GROUP, TOTAL, TOYOTA

New “Hydrogen Council” launched in Davos in Jan. 2017.

Alstom Coradia iLint:
The world's 1st hydrogen powered train

https://youtu.be/jKOmvY3X0uA

Shanghai magnetic levitation train

Japan maglev train breaks world speed record again

21 April 2015 | Asia

Share

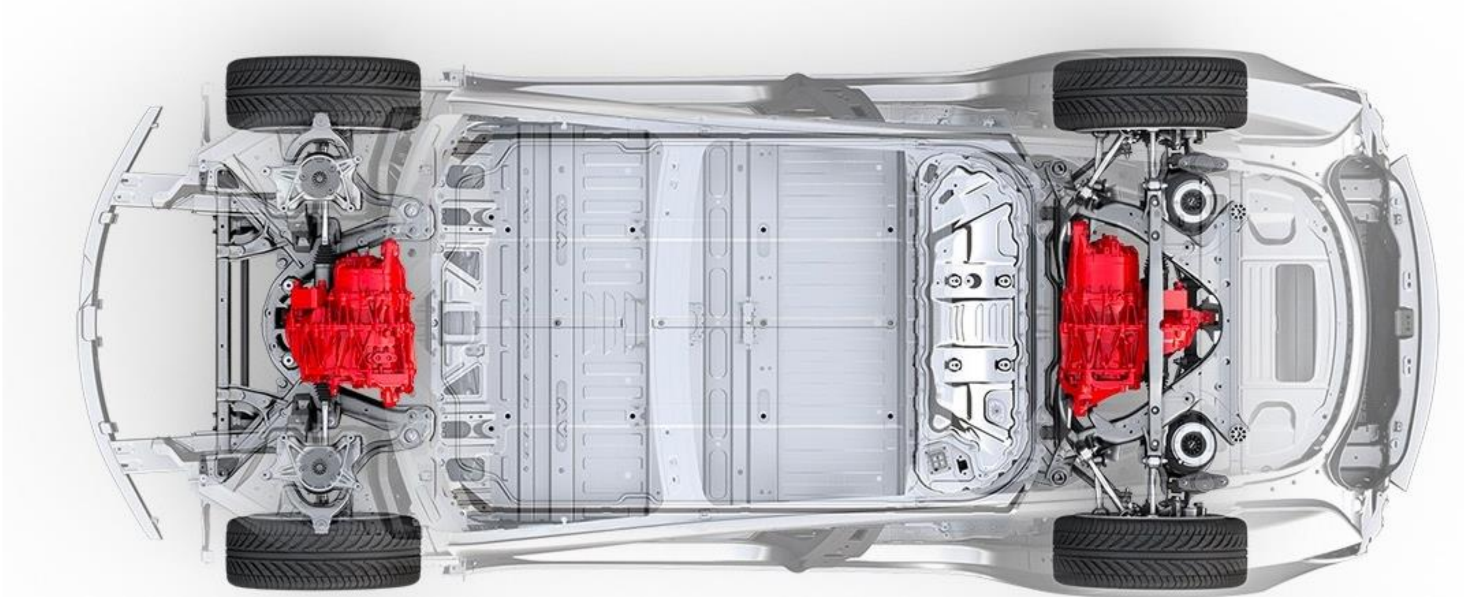
EPA

603 km/h (374 mph)

Quantum Levitation using superconductors

https://youtu.be/PXHczjOg06w

Permanent magnet electric motors



PERMANENT MAGNET TUNNEL THRUSTER

Reliable, efficient and low through life cost

The TT-PM is engineered and built with focus on reliability and efficiency. The core mechanical technology is well proven and verified through rigorous design processes, quality control, testing and verification.

Permanent magnet generators for wind turbines

Siemens Gamesa SG 14-236 DD

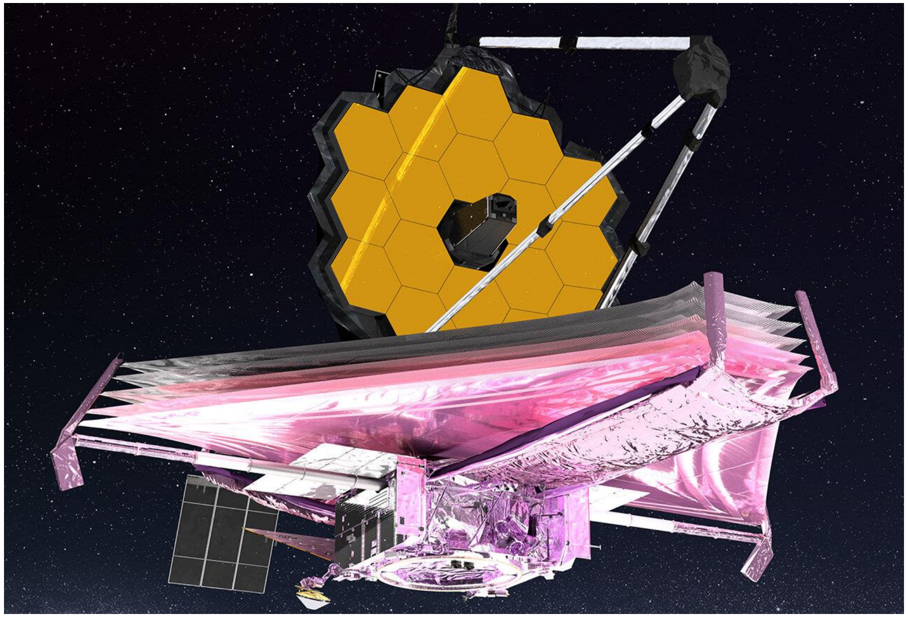
Rotor diameter: 236 m

Nominal power: 14 MW

https://www.siemensgamesa.com/products-and-services/offshore/wind-turbine-sg-14-236-dd

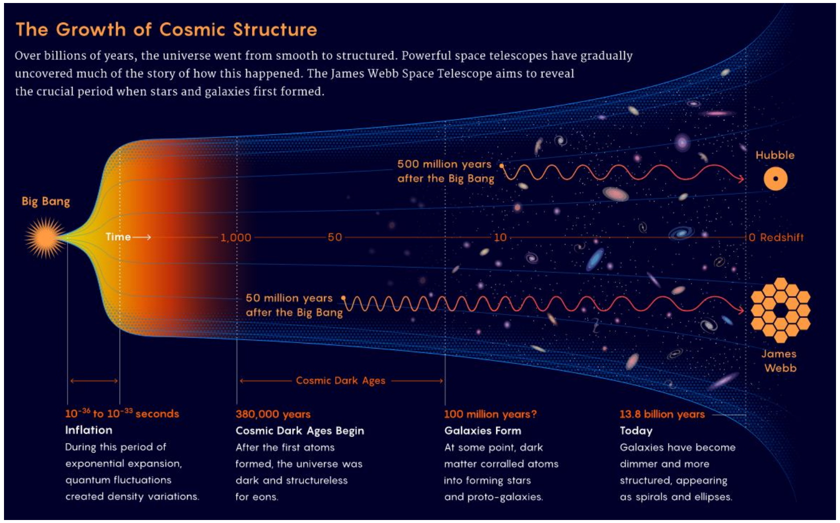
https://www.ge.com/news/reports/this-massive-magnet-will-generate-power-at-americas-first-offshore-windfarm

Piezoelectric actuators for James Webb Space Telescope



Launch date: 25 December 2021

Entered service: 12 July 2022



The Growth of Cosmic Structure

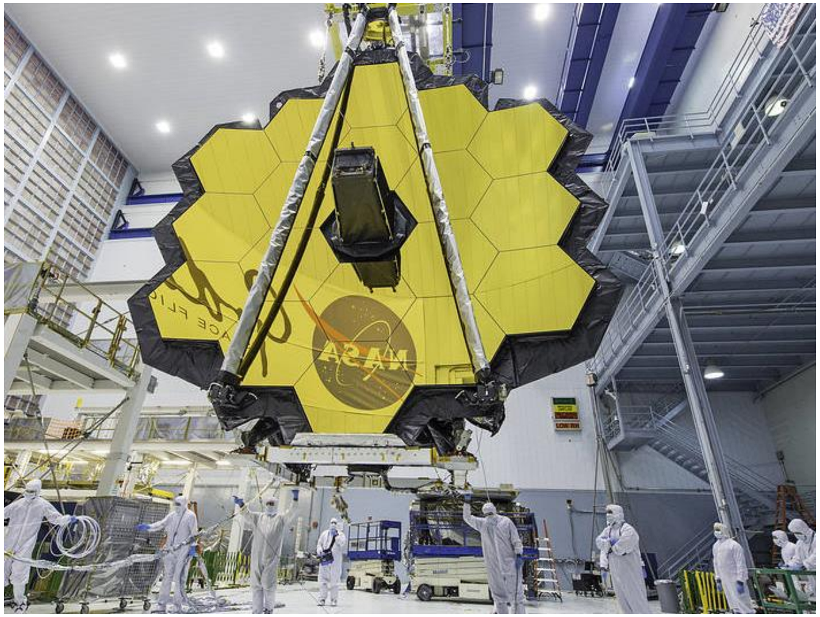
Over billions of years, the universe went from smooth to structured. Powerful space telescopes have gradually uncovered much of the story of how this happened. The James Webb Space Telescope aims to reveal the crucial period when stars and galaxies first formed.

10^{-36} to 10^{-33} seconds
Inflation
During this period of exponential expansion, quantum fluctuations created density variations.

380,000 years
Cosmic Dark Ages Begin
After the first atoms formed, the universe was dark and structureless for eons.

100 million years?
Galaxies Form
At some point, dark matter corralled atoms into forming stars and proto-galaxies.

13.8 billion years
Today
Galaxies have become dimmer and more structured, appearing as spirals and ellipses.



Diameter of primary mirror: 6.5 meter

18 hexagonal-shaped mirror segments that can be folded up to fit into a rocket.

Aligning the primary mirror segments using **piezoelectric actuators** to achieve a single perfect focus (‘*each mirror is aligned to 1/10,000th the thickness of a human hair*’).

https://webb.nasa.gov/content/observatory/ote/mirrors/index.html

https://www.quantamagazine.org/why-nasas-james-webb-space-telescope-matters-so-much-20211203/

Piezoelectric hexapod robots

https://youtu.be/jvmuHs-y1DQ

BLOCK 4: learning objectives

- To understand energy generation and storage materials/systems (fuel cells, batteries, supercapacitors).
- To understand the magnetic properties, hard and soft magnets and their applications.
- To understand the principles behind piezoelectrics and how they can be manipulated for materials design in different applications.
- To be able to perform material selection analysis based on analysis of operating conditions, material properties and other relevant factors including legislation.

BLOCK 4: Designing with Functional Materials

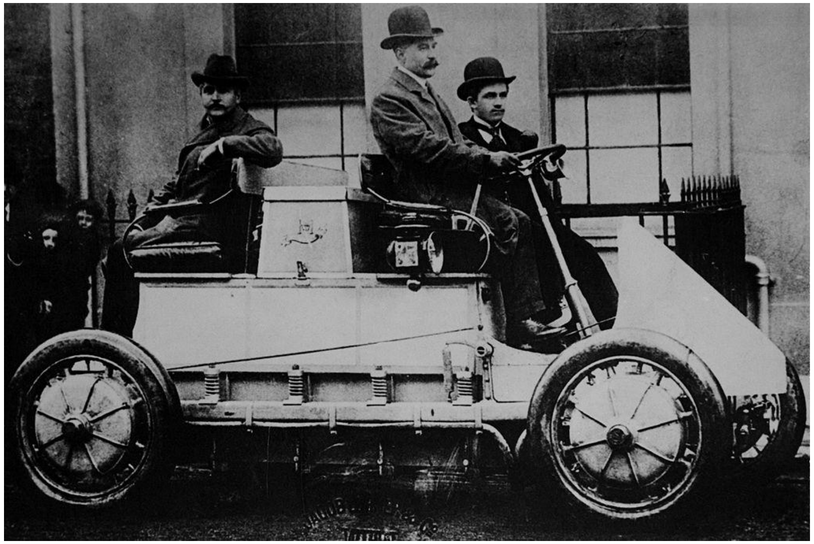
Case study: designing electric propulsion systems for road vehicles.

Desired properties:

1. High specific energy for long travel range
2. High specific power for fast acceleration
3. Low emission and pollution
4. Low cost
5. Short refilling/charging period
6. Low weight
7. High reliability
8. Long life span

Electrification of transport

Thomas Parker, who was born in Ironbridge, Shropshire, designed and built an electric car in Wolverhampton in 1884.



World's first hybrid electric car was invented by Ferdinand Porsche in 1901. The vehicle was powered by electricity stored in a battery and a gas engine.

Electric cars gained popularity.

Electric vehicles on Fifth Avenue in New York City during the 1910s.

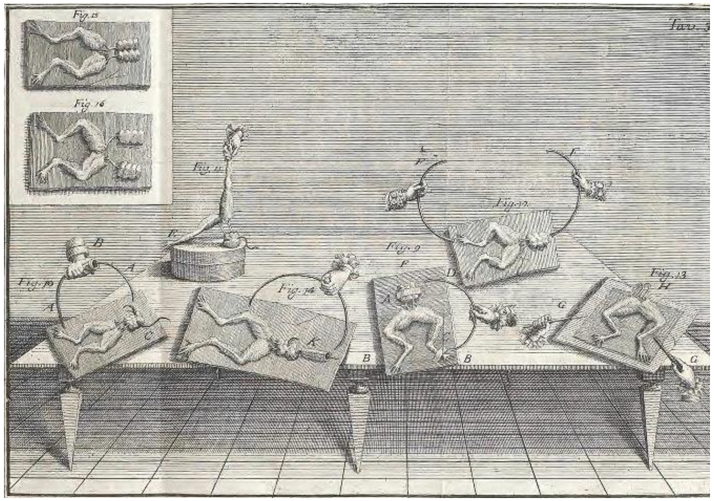
Better roads and discovery of cheap crude oil led to the decline in electric vehicles from 1920s.

Invention of batteries

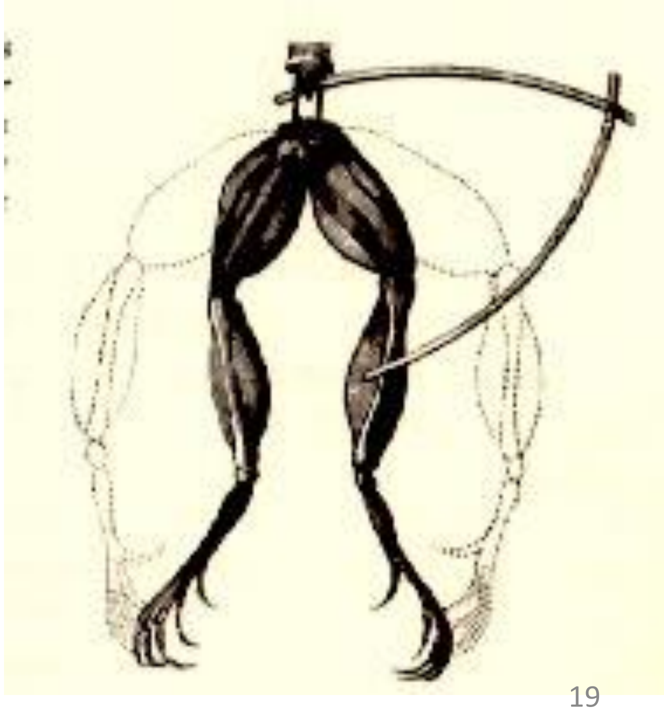
Luigi Galvani, ‘animal electricity’, 1791

The leg of a dead frog twitched when two different metals connected to the frog body touched.

Galvani believed this phenomenon was caused by ‘animal electricity’.



‘Commentary on the Effect of Electricity on Muscular Motion’ (‘De Viribus Electricitatis in Motu Musculari Commentarius’), 1791.



Invention of batteries

Alessandro Volta, ‘Volta pile’, ~1800

Volta however believed the electricity was produced by the two different metals used to connect the animal bodies rather than animals themselves.

Volta pile consists of alternating **copper (or silver**) and **zinc** disks separated by **brine-soaked pieces of cardboard or cloth**.

Tasting electricity

Put two coins made of different metals on the tip of tongue.

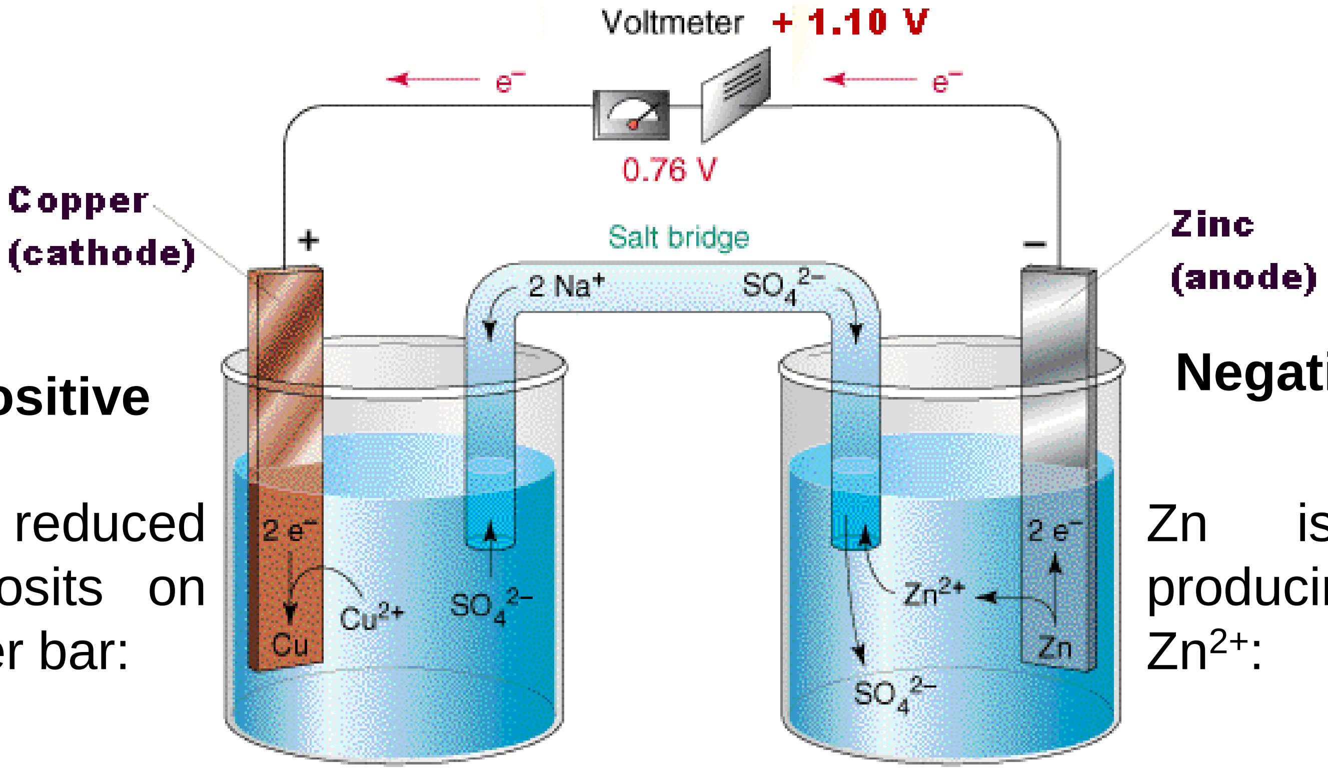
Then place a silver spoon on top of both coins.

Tingling sensation.

Volta demonstrating his battery to Napoleon in 1801

Working principle of batteries

John F. Daniell, ‘Daniell Battery’, 1836



Positive

Cu^{2+} is reduced and deposits on the copper bar:

Negative

Zn is oxidised, producing aqueous Zn^{2+}:

$Cu^{2+} (aq) + 2e^{-} \rightarrow Cu (s)$

Reduction reaction (gaining electrons)

$Zn (s) \rightarrow Zn^{2+} (aq) + 2e^{-}$

Oxidation reaction (losing electrons)

The total reaction: **$Zn (s) + Cu^{2+} (aq) \rightarrow Zn^{2+} (aq) + Cu (s)$**

http://chemwiki.ucdavis.edu/Analytical_Chemistry/Electrochemistry/Electrochemistry_2%3A_Galvanic_cells_and_Electrodes

Working principle of batteries

The standard cell potential, $\mathbf{E^0_{cell}}$, is determined by change of the standard Gibbs free energy for the chemical reaction according to:

$$\Delta G^0 = -nFE^0_{cell}$$

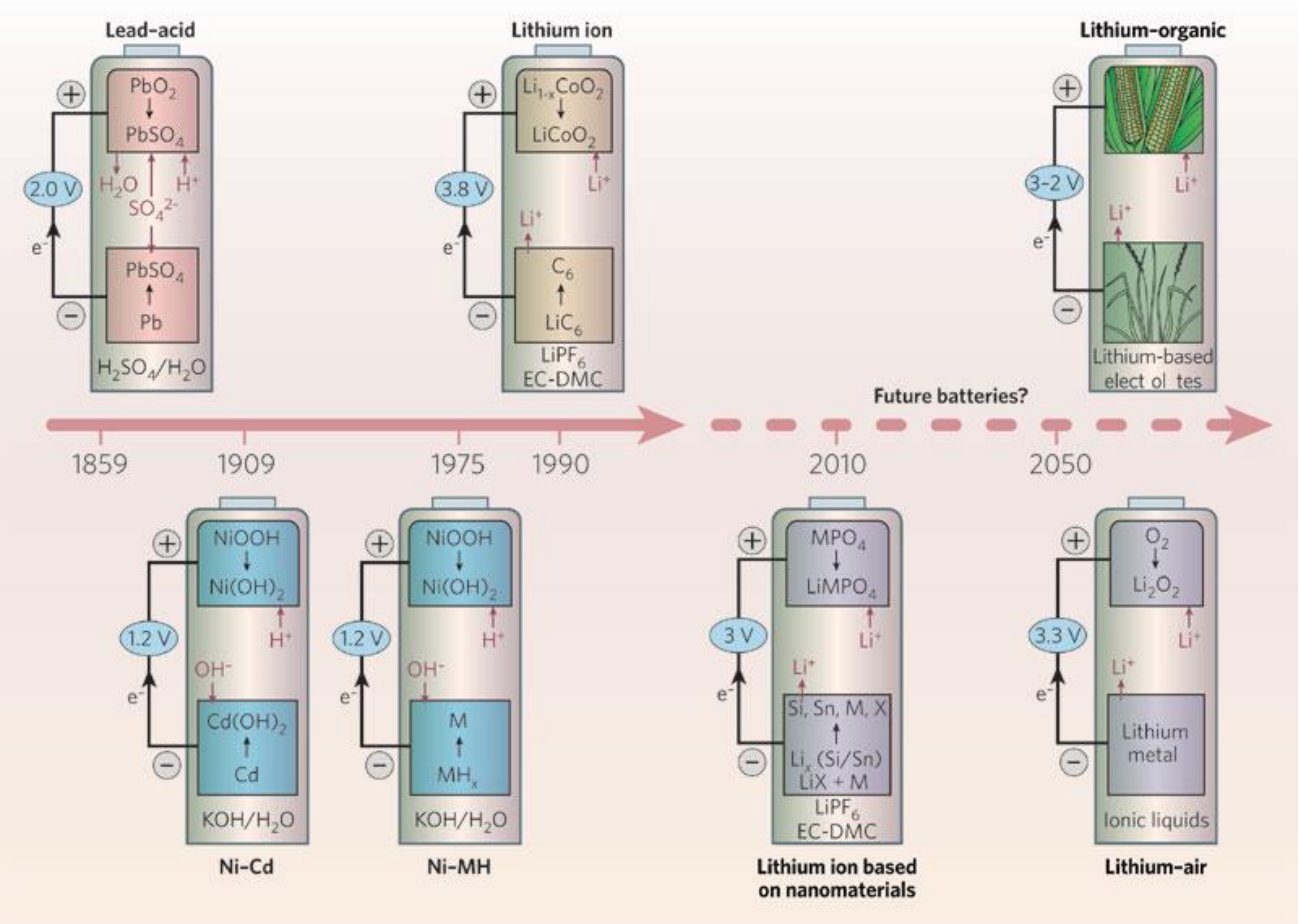
F is the Faraday constant 96,485 C/mol

n is the number of electrons transfered per mole of reaction

Chemical energy is directly converted to electricity through oxidation and reduction reactions → high energy conversion efficiency.

Standard condition:

- ☐ Activities of all reactants and products are unity (all equal to 1).
- ☐ The pressure of any gaseous component is 1 bar (10^5 Pa)
- ☐ Unit activity for a solid component
- ☐ T = 298 K



M. Armand & J.M. Tarascon, Building better batteries, Nature 2008, **51**, 652-657.

Lead-Acid Battery

Invented by Gaston Planté, 1859.

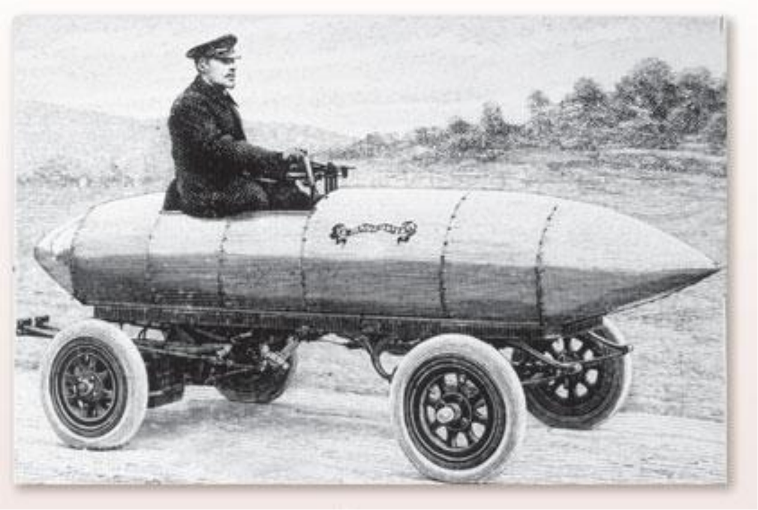
First rechargeable (secondary type) battery

Most commonly used for:

Starting, Lighting and Ignition (SLI) applications

Stand-by (stationary) backup power applications.

Lead acid battery vehicles



M. Armand & J.M. Tarascon, Building better batteries, Nature 2008, **51**, 652-657.

In 1899 a Belgian car powered by a lead–acid battery pack reached a speed of 100 km/h.

General Motors EV1 (1996-1999)
Powered by a 16.5 kWh lead-acid battery with a mass of 533 kg and can travel up to ~ 60 miles per full charge.
The specific energy 16.5 kWh/533 kg = **31 Wh/kg** is low, limiting travel range.

Lead-Acid Battery

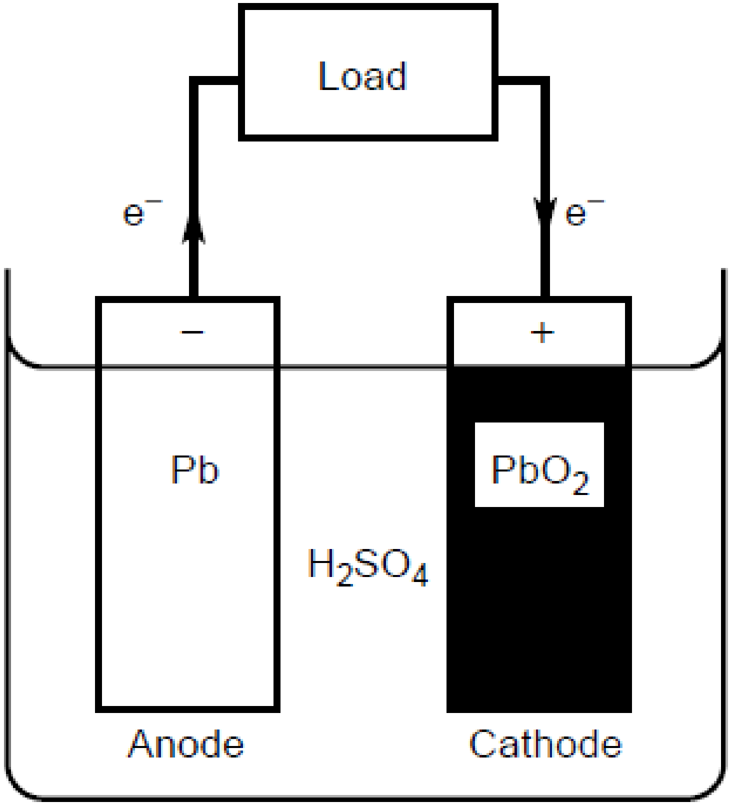
Negative electrode: $Pb(s) + SO_4^{2-}(aq) \rightleftharpoons PbSO_4(s) + 2e^-$ **($E^0 = -0.36$ V)**

Positive electrode:

$PbO_2(s) + 4H^+ + SO_4^{2-} + 2e^- \rightleftharpoons PbSO_4(s) + 2H_2O(l)$ **($E^0 = 1.69$ V)**

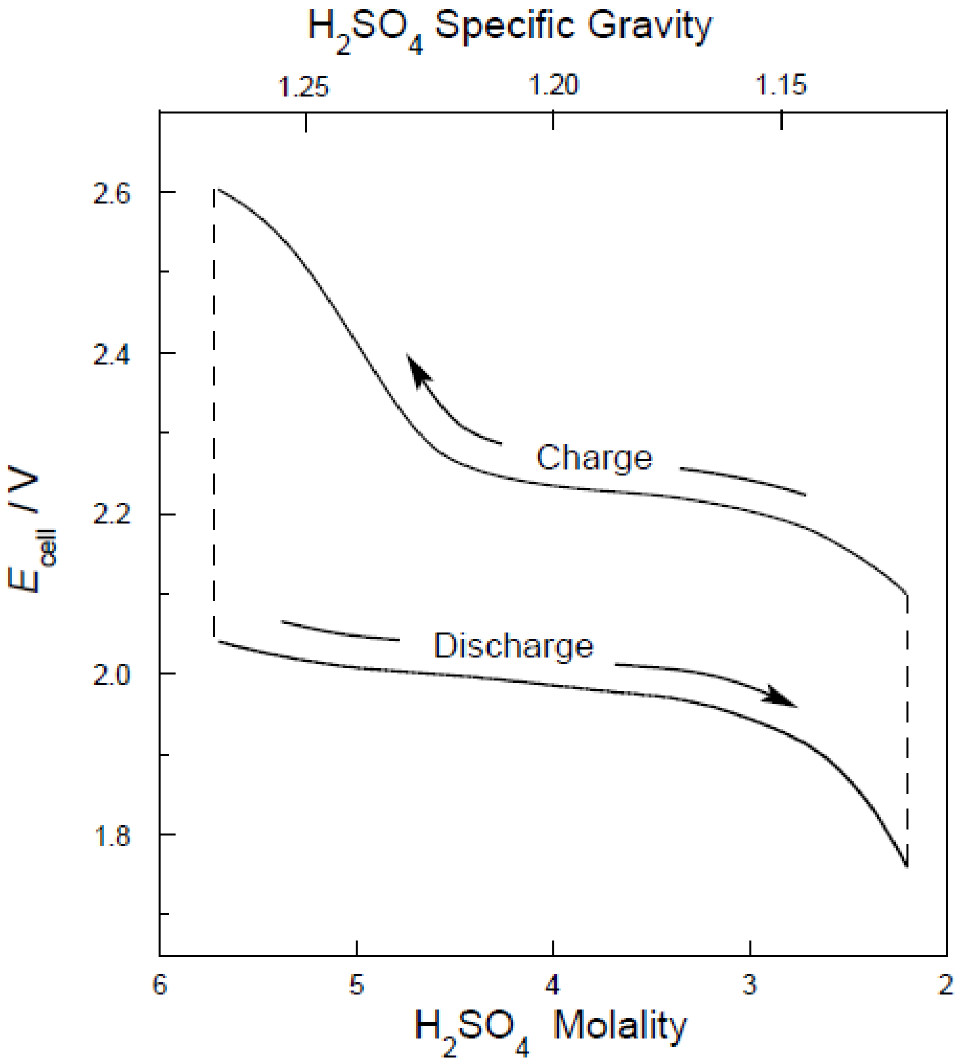
Overall: $PbO_2(s)+Pb(s)+2H_2SO_4(aq) \rightleftharpoons 2PbSO_4(s) + 2H_2O(l)$

$E^0_{cell} = 1.69\text{ V} – (-0.36\text{ V}) = 2.05\text{ V}$



R.S. Treptow, *J. Chem. Edu*, 2002, **79**, 334

E_{cell} depends on H_2SO_4 concentration.



R.S. Treptow, *J. Chem. Edu*, 2002, **79**, 334

The key performance parameters

Specific Energy (Wh/kg) – The nominal battery energy per unit mass, sometimes referred to as the gravimetric energy density.

Specific Power (W/kg) – The maximum available power per unit mass.

Energy Density (**Wh/L**) – The nominal battery energy per unit volume, sometimes referred to as the volumetric energy density.

Power Density (W/L) – The maximum available power per unit volume.

1 Ah = 1 Amp*hour = 1 C/s * 3600s = 3600 C

1 Wh = 1 J/s * 3600s = 3600 J

Calculating theoretical specific capacity and specific energy

For lead-acid battery:

$PbO_2(s) + Pb\ (s) + 2\ H_2SO_4\ (aq) \rightleftharpoons 2\ PbSO_4\ (s) + 2H_2O\ (l)$

n=2. The sum of the **molecular weight, MW**, of the reactants (PbO_2 + Pb + 2 H_2SO_4) is **643 g mol^{-1}** (other components are ignored here)

$$\text{Specific capacity} = \frac{nF}{[3600\ \text{C/Ah} * \text{MW}]} = \frac{2 * 96485\ \text{C/mol}}{[3600\ \text{C/Ah} * 643\ \text{g/mol}]}$$

$$= 0.0833\ \text{Ah/g} = 83\ \text{mAh/g}$$

$$\text{Specific energy} = \frac{nFE^{o}_{cell}}{[3600\ \text{J/Wh} * \text{MW}]} = \frac{2 * 96485\ \text{C/mol} * 2.05\ \text{V}}{[3600\ \text{J/Wh} * 643\ \text{g/mol}]}$$

$$= 0.171\ \text{Wh/g} = 171\ \text{Wh/kg}$$

Practical specific energy is much lower than the theoretical value

Voltage: 12 V Capacity: 41 Ah

Mass: 11.80 kg

Specific energy = (12 V × 41 Ah) / 11.8 kg
=**41.7 Wh/kg**

Theoretical specific energy: **171 Wh/kg**

Low utilisation efficiency of the active mass (electrolyte and electrode materials) and the weight of peripheral materials (e.g., water, grid metal, separators, connectors, terminals, cell container).

Lead-Acid Battery

- ☐ Wide range of operation temperature range
- ☐ Perform well on high load currents
- ☐ Mature manufacturing technology
- ☐ **Low price**

Lead Acid 12V Car Battery: £50-100.

- ☐ Low specific energy (30-40 Wh/kg)
- ☐ Limited cycle life, do not like full discharges
- ☐ Must be stored with sufficient charge
- ☐ Produce gases, need ventilation
- ☐ Environmentally unfriendly (lead is a highly toxic metal)

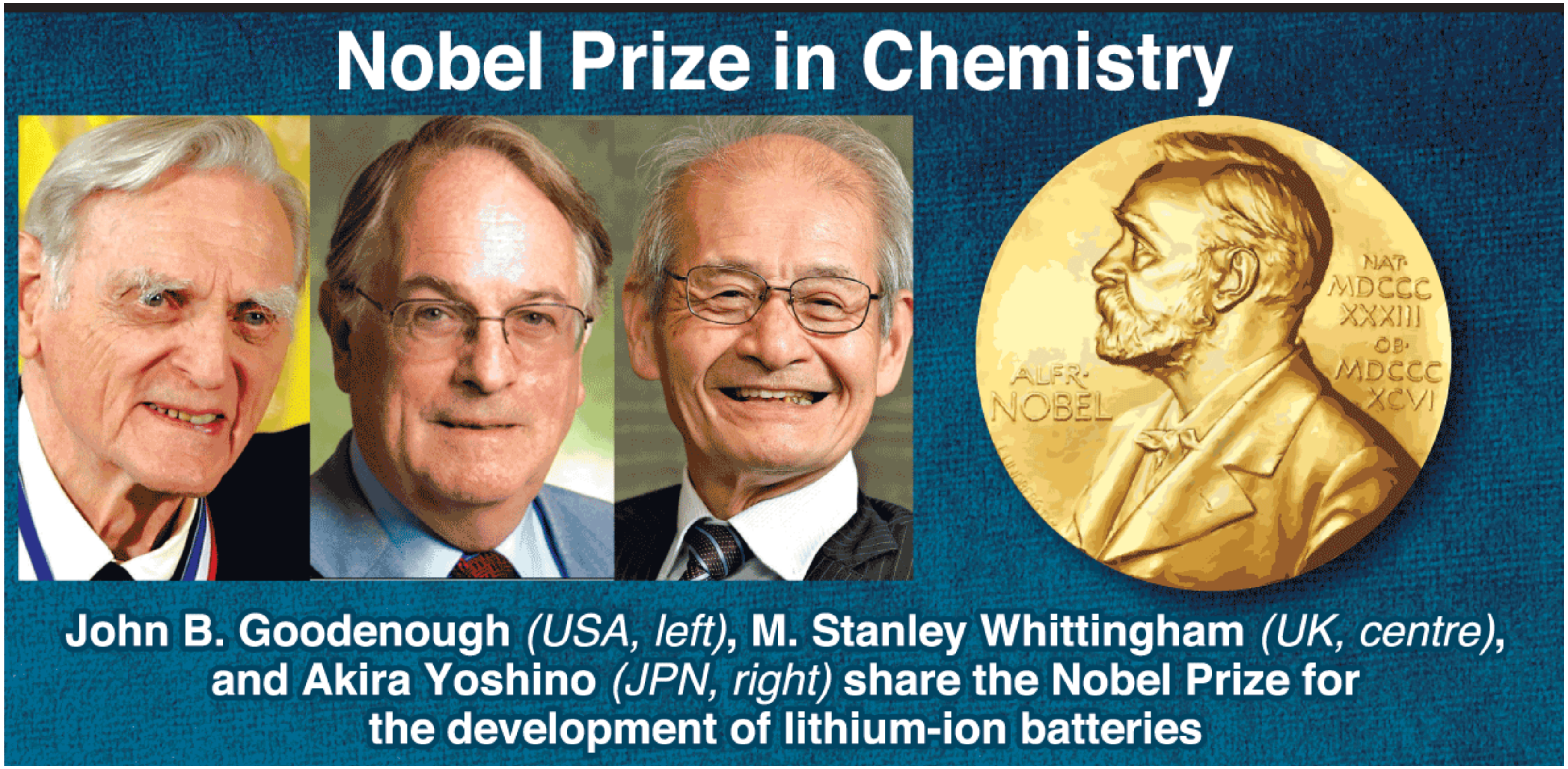
Lithium ion 12 V battery: £300-500.

Lead acid batteries are relatively cheap and reliable, and therefore still commonly used in vehicle SLI applications

Lithium ion batteries for a rechargeable world

The Nobel Prize in Chemistry 2019

“for the development of lithium-ion batteries”



Nobel Prize in Chemistry

John B. Goodenough *(USA, left)*, **M. Stanley Whittingham** *(UK, centre)*, **and Akira Yoshino** *(JPN, right)* **share the Nobel Prize for the development of lithium-ion batteries**

Lithium ion battery

Negative electrode:

LiC_6 (s) → 6C (s) + Li^+ + e^-

Positive electrode:

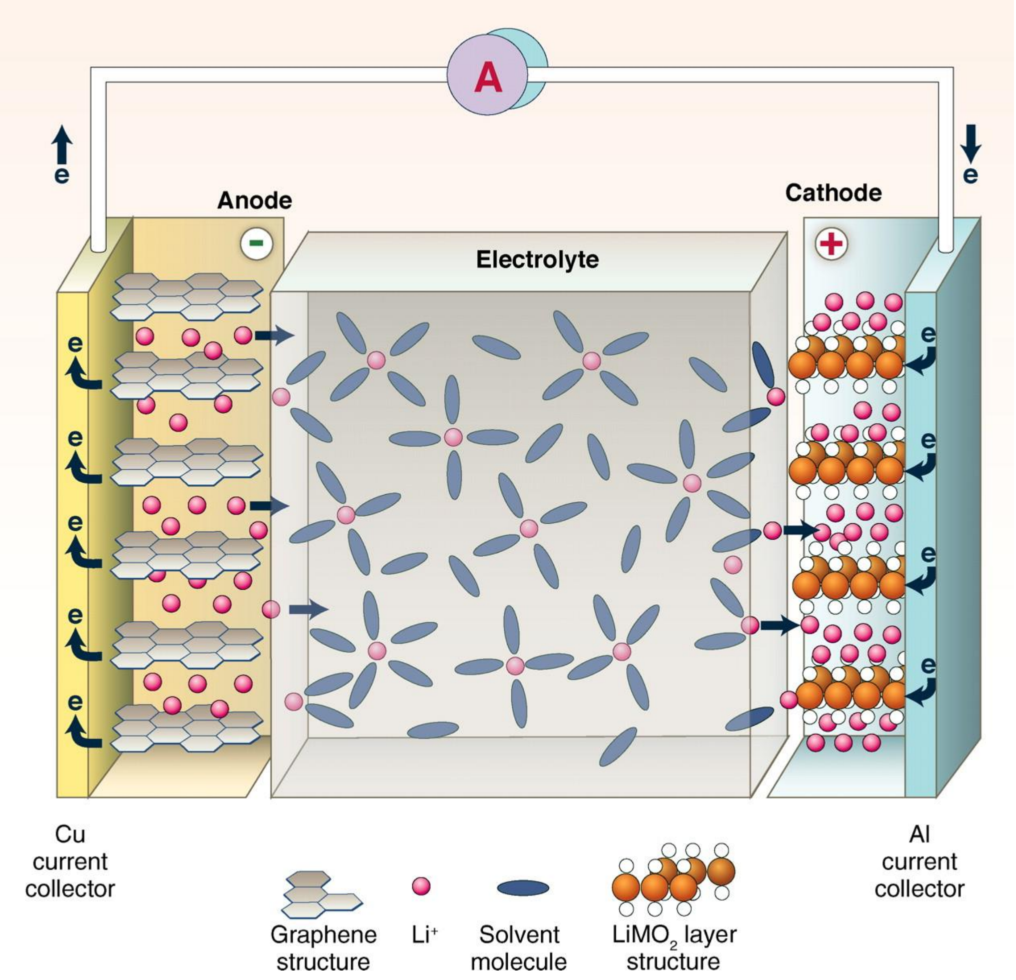
$FePO_4$ (s) + Li^+ + e^- → $LiFePO_4$ (s)

Overall:

LiC_6 (s) + $FePO_4$ (s) → 6C (s) + $LiFePO_4$ (s)

During charge, lithium ions are extracted from $LiFePO_4$, diffuse through the electrolyte, and are intercalated between the graphite sheets (negative electrode).

During discharge, Li ions return to the positive electrode via the electronically insulating electrolyte, and electrons pass around the external circuit.



Bruce Dunn, Haresh Kamath, Jean-Marie Tarascon, Science 2011, **334**, 928-935.

Lithium ion battery

$LiCoO_2$, practical specific capacity and energy are 50-60% of theoretical values.

Positive electrode: $Li_{1-x}CoO_2 + x\ Li^+ + xe^- = LiCoO_2$

Negative electrode: $Li_xC_6 = x\ Li^+ + 6C + xe^-$

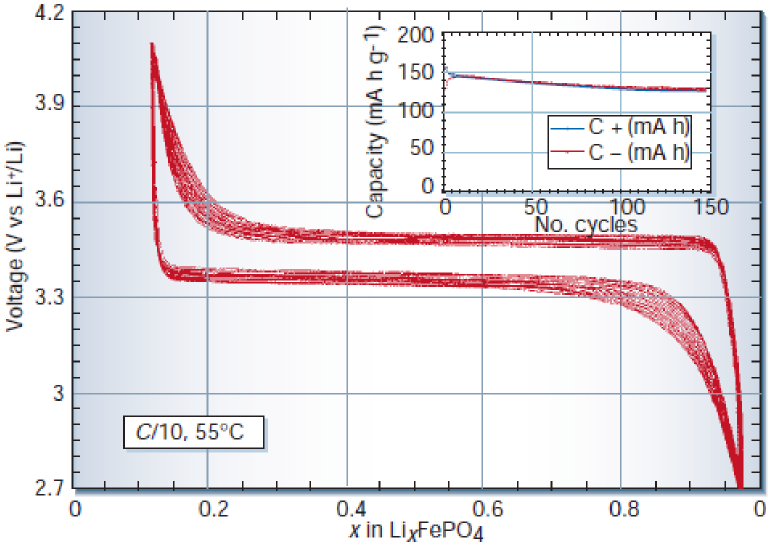
Cell: $Li_{1-x}CoO2 + Li_xC6 = LiCoO_2 + 6C$

($x < 1$)

$LiCoO_2$ was developed in 1980s and was commercialised by Sony in 1991.

Co is toxic and expensive.

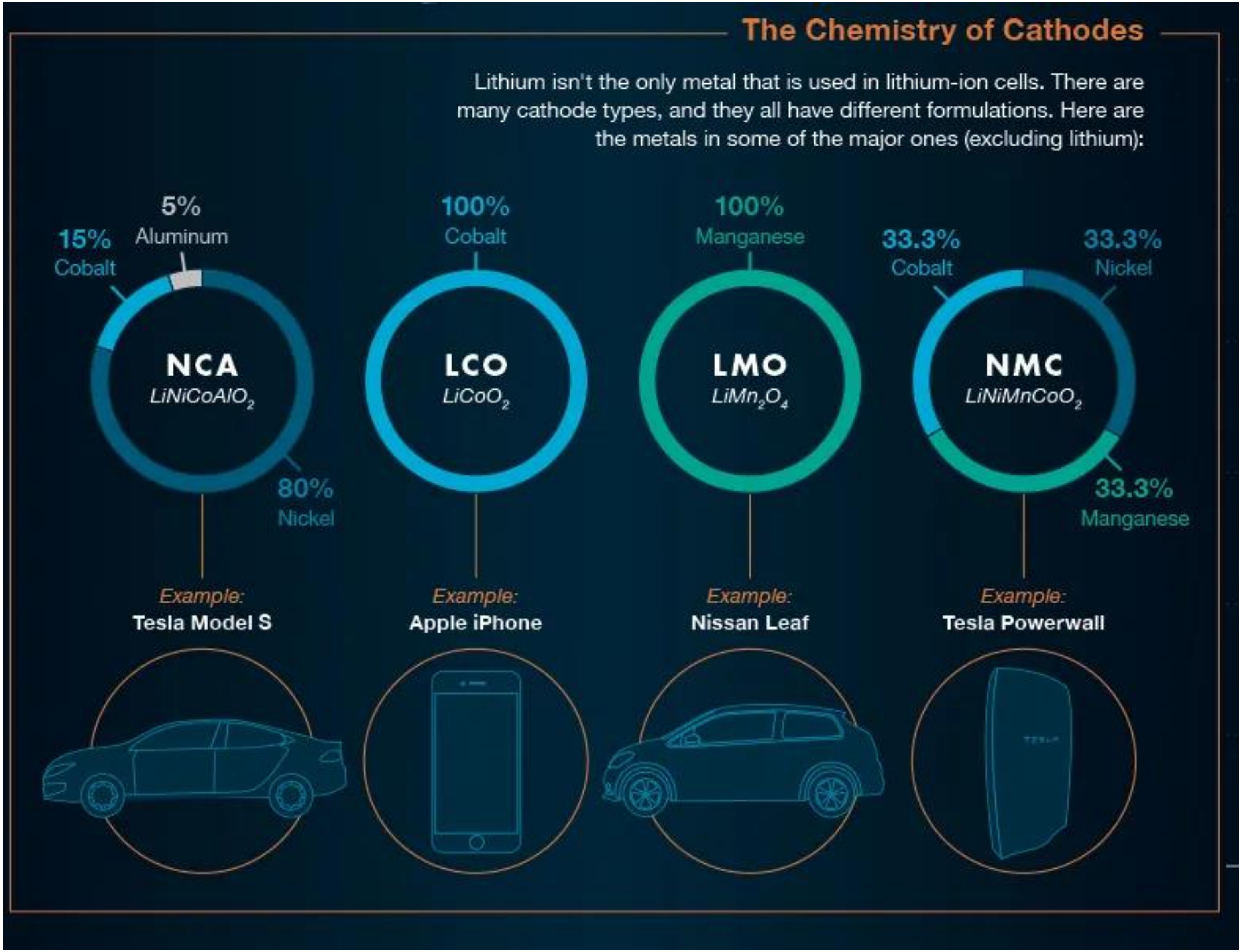
$LiFePO_4$: high stability, low cost and high compatibility with environments and can be used at 90% of its theoretical capacity.



J.M. Tarascon and M. Armand, Nature, 2001, **414**, 359-367.

Common commercial cathode materials for lithium ion batteries

Cathode materials	Chemical formula	Nominal voltage (V)	Specific energy (Wh/kg)
Lithium Cobalt Oxide	$LiCoO_2$ (**LCO**)	3.60	150-200
Lithium Manganese Oxide	$LiMn_2O_4$ (**LMO**)	3.80	100-150
Lithium Nickel Manganese Cobalt Oxide	$LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (**NMC**)	3.70	150-220
Lithium Iron Phosphate	$LiFePO_4$ (**LFP**)	3.30	90-120
Lithium Nickel Cobalt Aluminium Oxide	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (**NCA**)	3.60	200-260

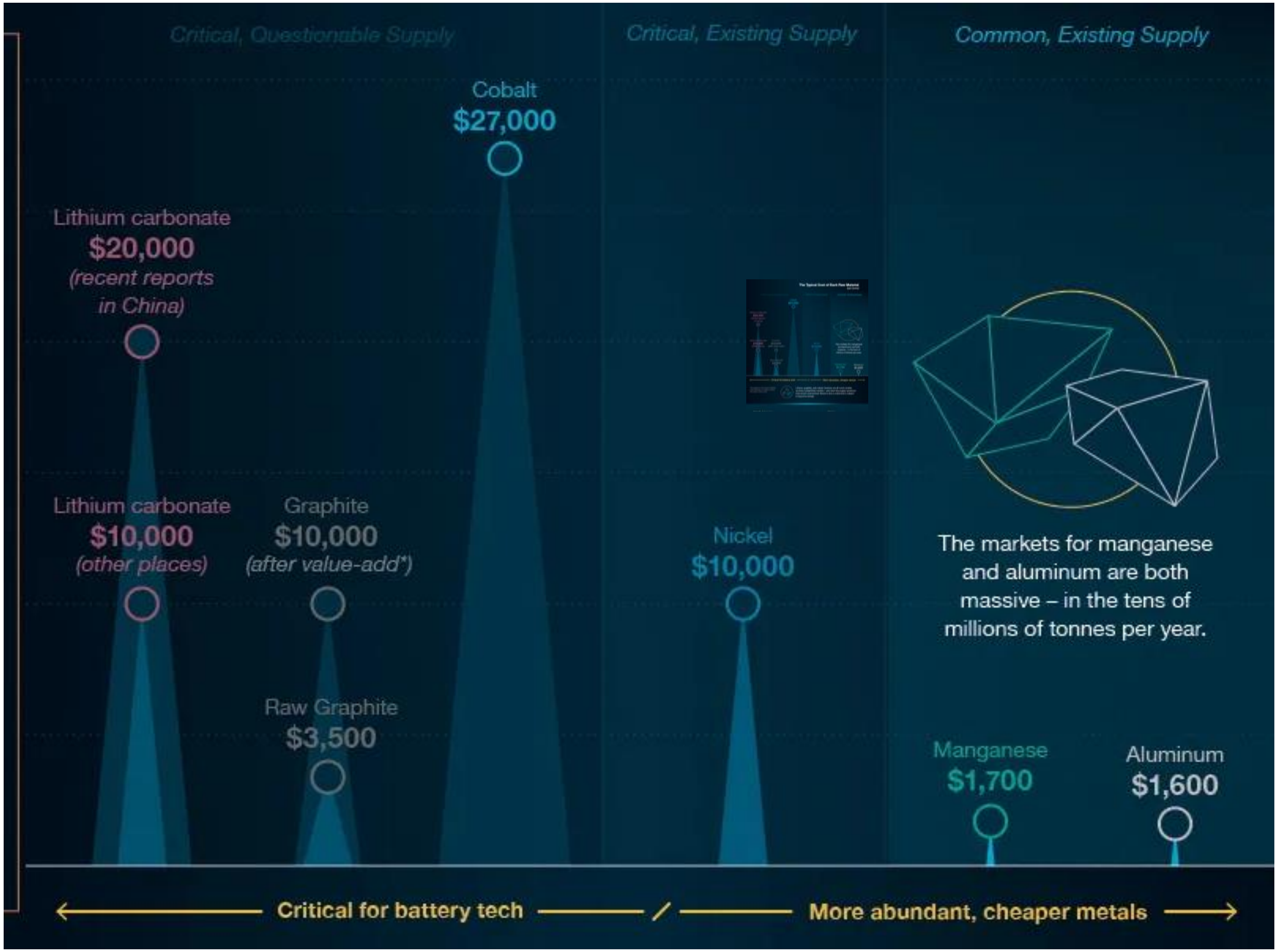


The Chemistry of Cathodes

Lithium isn't the only metal that is used in lithium-ion cells. There are many cathode types, and they all have different formulations. Here are the metals in some of the major ones (excluding lithium):

https://www.visualcapitalist.com/critical-ingredients-fuel-battery-boom/

Typical costs of raw materials per ton



The markets for manganese and aluminum are both massive – in the tens of millions of tonnes per year.

https://www.visualcapitalist.com/critical-ingredients-fuel-battery-boom/

Exercise

Molecular Weight of $LiCoO_2$ = 97.9 g mol^{-1} and $\mathbf{LiFePO_4}$ = 157.8 g mol^{-1}

Theoretical specific capacity of $LiCoO_2$ and $\mathbf{LiFePO_4}$?

Theoretical specific energy of $LiCoO_2$ and $\mathbf{LiFePO_4}$?

1 Ah = 1 Amp*hour = 1 C/s * 3600s = 3600 C

1 Wh = 1 J/s * 3600s = 3600 J

$$\text{Specific capacity} = \frac{nF}{[3600\ \text{C/Ah} * \text{MW}]} = \frac{1 * 96485\ \text{C/mol}}{[3600\ \text{C/Ah} * 157.8\ \text{g/mol}]}$$

$$= 0.170\ \text{Ah/g} = 170\ \text{mAh/g}$$

$$\text{Specific energy} = \frac{nFE}{[3600\ \text{J/Wh} * \text{MW}]} = \frac{1 * 96485\ \text{C/mol} * 3.3\ \text{V}}{[3600\ \text{J/Wh} * 157.8\ \text{g/mol}]}$$

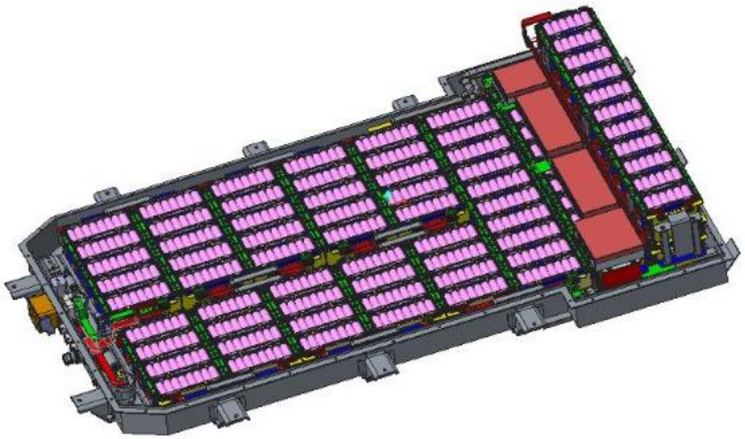
$$= 0.560\ \text{Wh/g} = 560\ \text{Wh/kg}$$

Lithium ion battery 18650 vs 21700

Samsung SDI batteries – 18650 vs 21700

- **Nominal capacity**: 4,750 mAh
- **Nominal voltage**: 3.6 V
- **Max. weight**: 75 g
- **Life cycle**: 80 % at 500 charge/discharge cycles
- **Dimension**: 21×70 mm
- **Gravimetric energy density**: 228 Wh/kg
- **Volumetric energy density:** 705 Wh/L

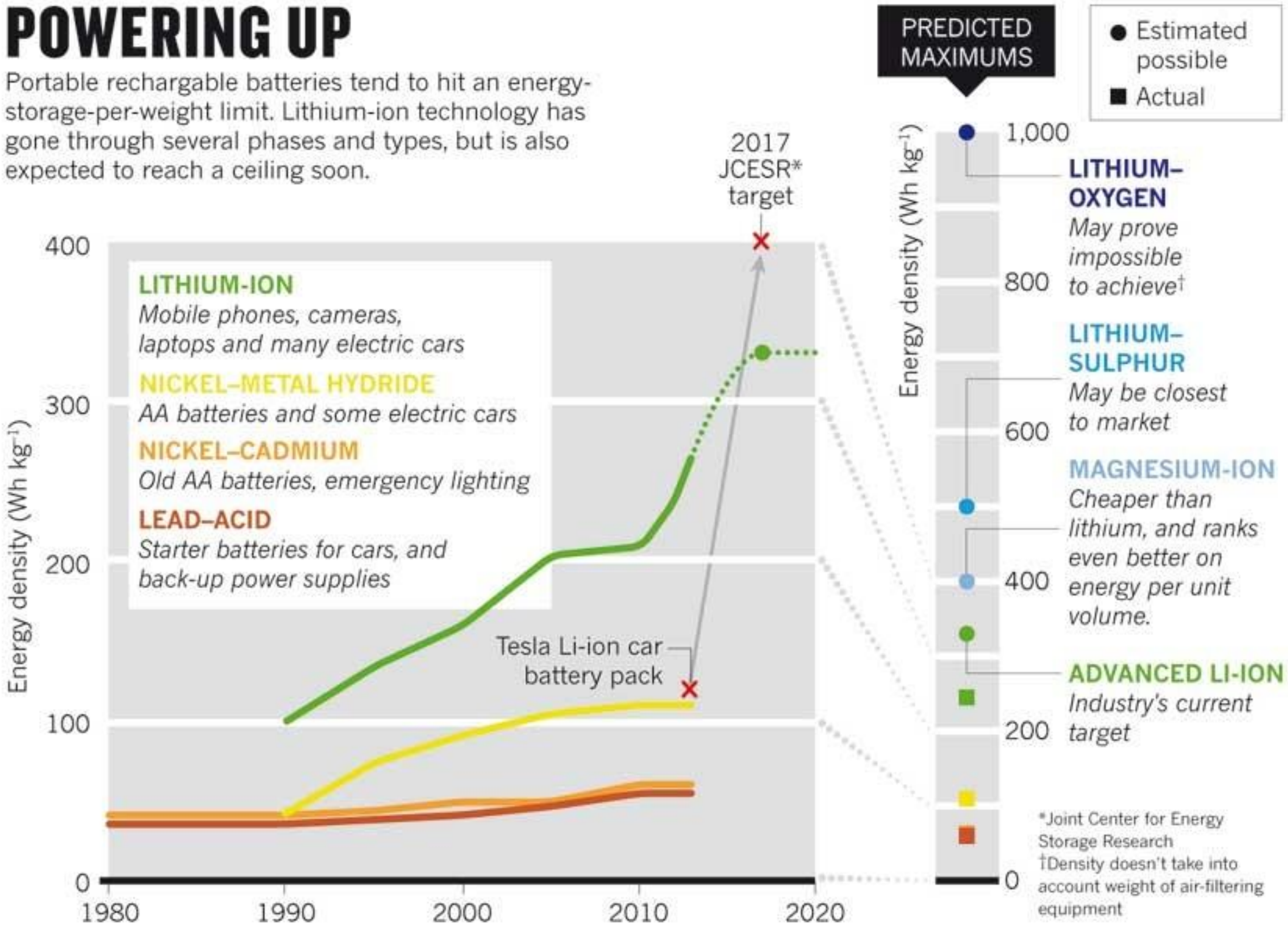
Tesla uses 8,256 cells across the 16 modules per P100D battery pack with 102.4 kWh total capacity.



https://pushevs.com/2017/03/15/technology-regulation-motivation/
https://www.dnkpower.com/the-future-will-be-21700/

Challenges for electric vehicles?

Higher specific energy is needed.



POWERING UP

Portable rechargable batteries tend to hit an energy-storage-per-weight limit. Lithium-ion technology has gone through several phases and types, but is also expected to reach a ceiling soon.

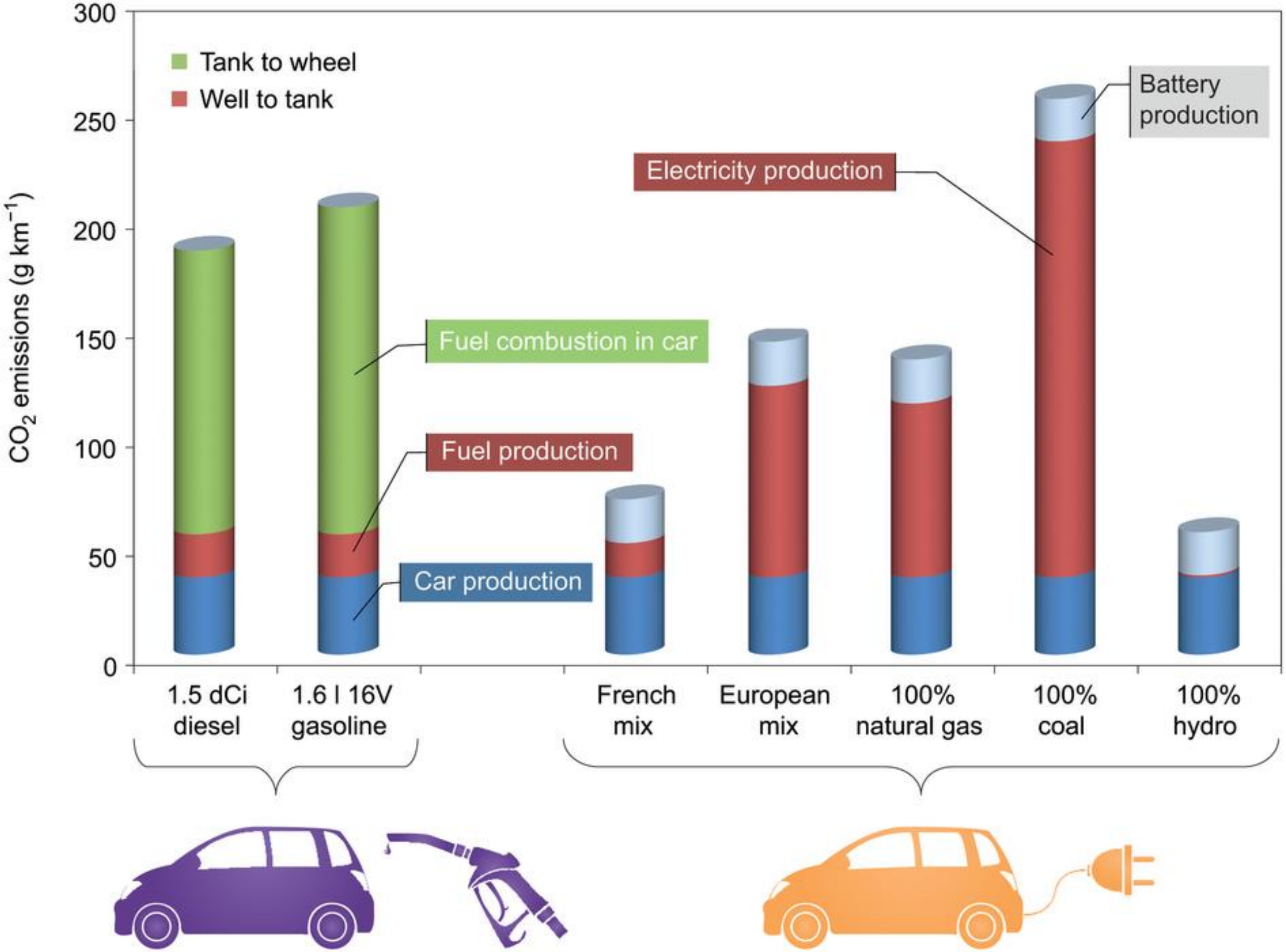
*Joint Center for Energy Storage Research

†Density doesn't take into account weight of air-filtering equipment

Richard Van Noorden, The rechargeable revolution: a better battery, Nature 2014, **507**, 26–28.

Challenges for electric vehicles?

Really?

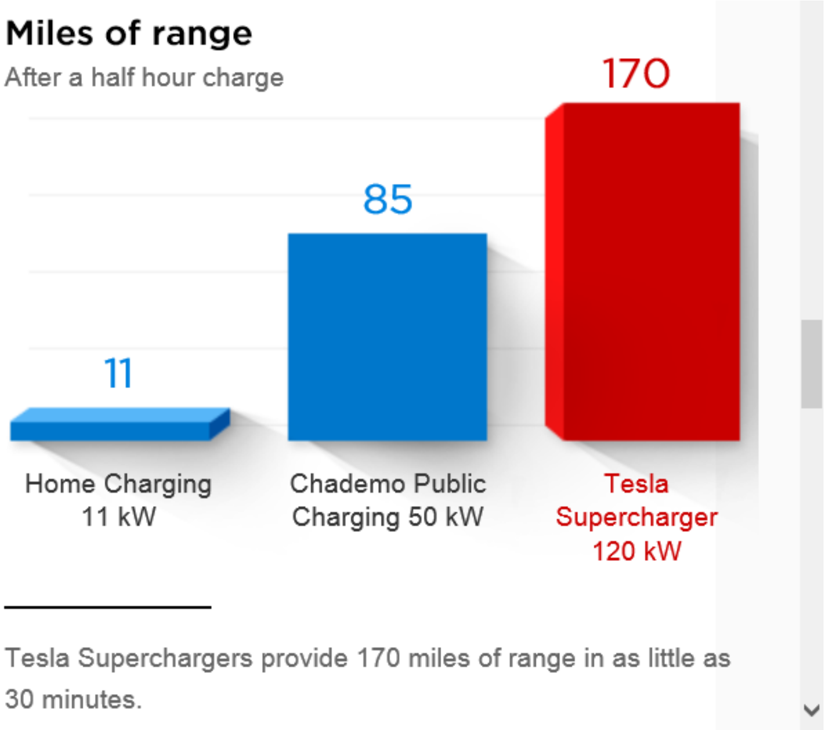


The CO$_2$ benefit of electric vehicles relies heavily on the origin of the electricity.

Nature Chemistry, 2015, **7**, 19–29.

Total CO$_2$ emissions (gkm^{-1}) for internal combustion engine cars (left) and for full electric vehicles (right) with various electricity origins. We assumed that electric vehicles are used at a rate of 10,000 km yr^{-1}, powered by Li-ion batteries (20 kWh pack, 8-yr lifespan) and consume 20 kWh per 100 km. The main contributors of the European electricity mix are: fossil fuels and waste combustion (53%), nuclear (25%) and renewable energies (hydro, wind, 21%). The main contributors of the French electricity mix are: nuclear (80%), renewable energies (hydro, wind, 11%), and fossil fuels and waste combustion (9%). The 'well to tank' step refers to the fuel production and delivery while the 'tank to wheel' step deals with the car operation (fuel combustion).

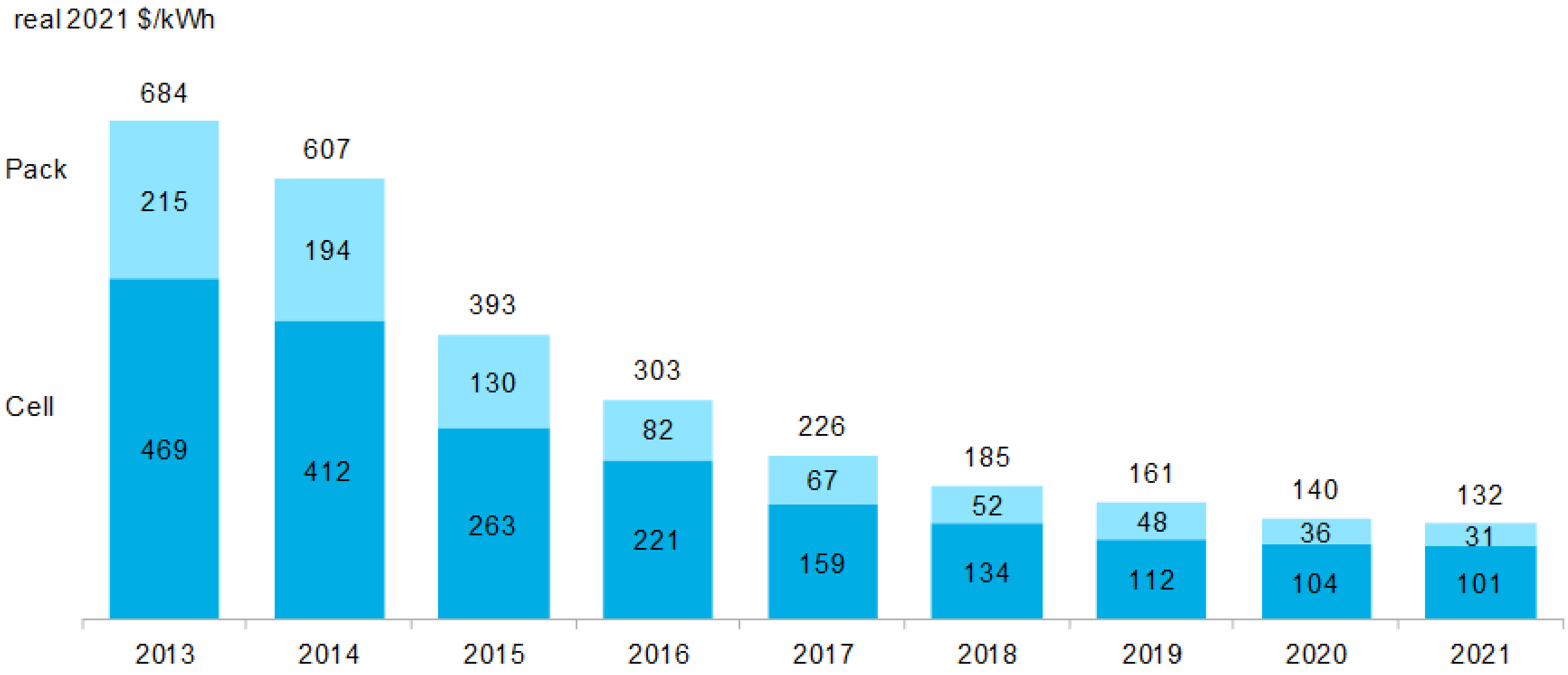
Challenges for electric vehicles?



Tesla Superchargers provide 170 miles of range in as little as 30 minutes.

Challenges for electric vehicles?

Figure 1: Volume-weighted average pack and cell price split



Source: BloombergNEF.

Key points：

- Working principle of batteries.
- How to calculate the specific capacity and specific energy for batteries.
- Ballpark figures of specific energy of lead-acid and lithium-ion batteries.
- The advantages and disadvantages of lead-acid and lithium-ion batteries.

Hydrogen fuel cell cars, buses and trains

Hyundai ix35

Toyota Mirai

Honda Clarity

Alstom train Coradia iLint

First test run in March 2017 in Germany.

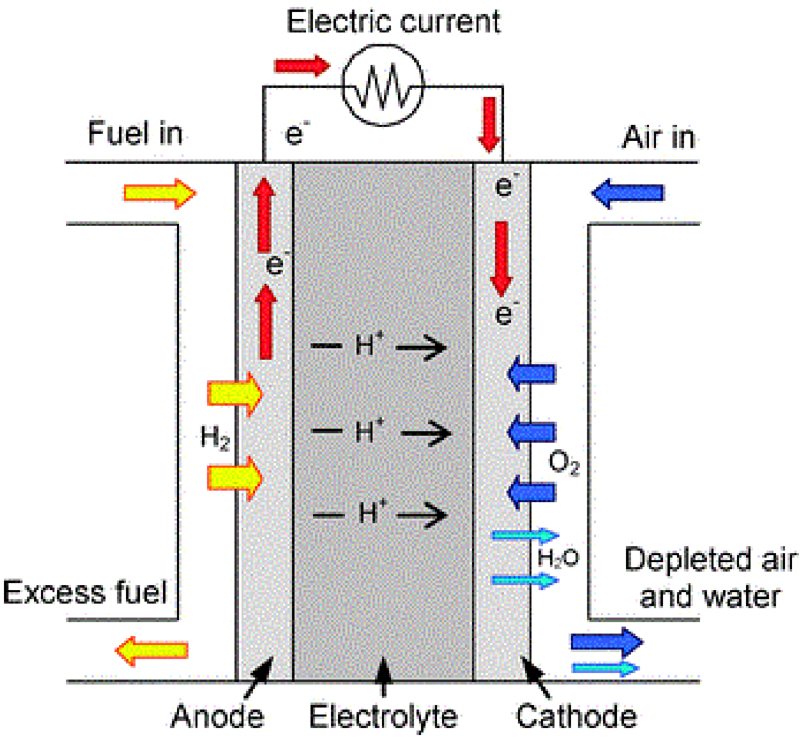
Entered service in Sep. 2018

AIR LIQUIDE Creative Oxygen ALSTOM AngloAmerican BMW GROUP DAIMLER engie by people for people

HONDA HYUNDAI Kawasaki THE LINDE GROUP TOTAL TOYOTA

New "Hydrogen Council" launched in Davos in Jan. 2017.

Proton exchange membrane fuel cell (PEMFC)



Schematic diagram of a PEMFC (Chem. Soc. Rev., **39** 4370, 2010).

Three main components :

Anode: porous carbon coated with tiny particles of platinum, responsible for splitting hydrogen into protons and electrons. $\mathbf{H_2 \rightarrow 2H^+ + 2e^-}$

Cathode: porous carbon coated with tiny particles of platinum, responsible for oxygen reduction by reacting with protons, generating electricity and water.

$\mathbf{1/2O_2 + 2H^+ + 2e^- \rightarrow H_2O}$

Overall: $\mathbf{H_2 + 1/2O_2 \rightarrow H_2O}$

Electrolyte*:* **proton exchange membrane** (PEM, proton conductor)

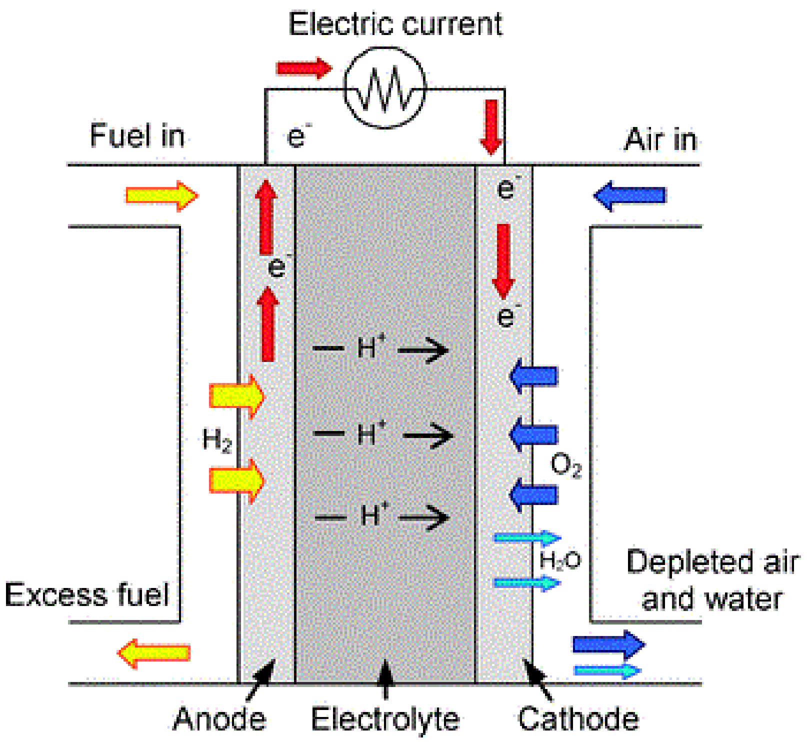
typically **DuPont Nafion®** membranes

Operation temperature ~ 80 °C.

High purity H_2 is used as fuel.

Proton exchange membrane fuel cells

PEMFCs



Schematic diagram of a PEMFC (Chem. Soc. Rev., **39** 4370, 2010).

Anode: $H_2 \rightarrow 2H^+ + 2e^-$

Cathode: $1/2O_2 + 2H^+ + 2e^- \rightarrow H_2O$

Overall: $\mathbf{H_2 + 1/2O_2 \rightarrow H_2O}$

$\Delta G = \Delta H - T\,\Delta S$

Where G is Gibbs free energy,

H is enthalpy, S is entropy

$\Delta H = -\ 286$ kJ/mol

$\Delta G = -\ 237$ kJ/mol

T = 273 K

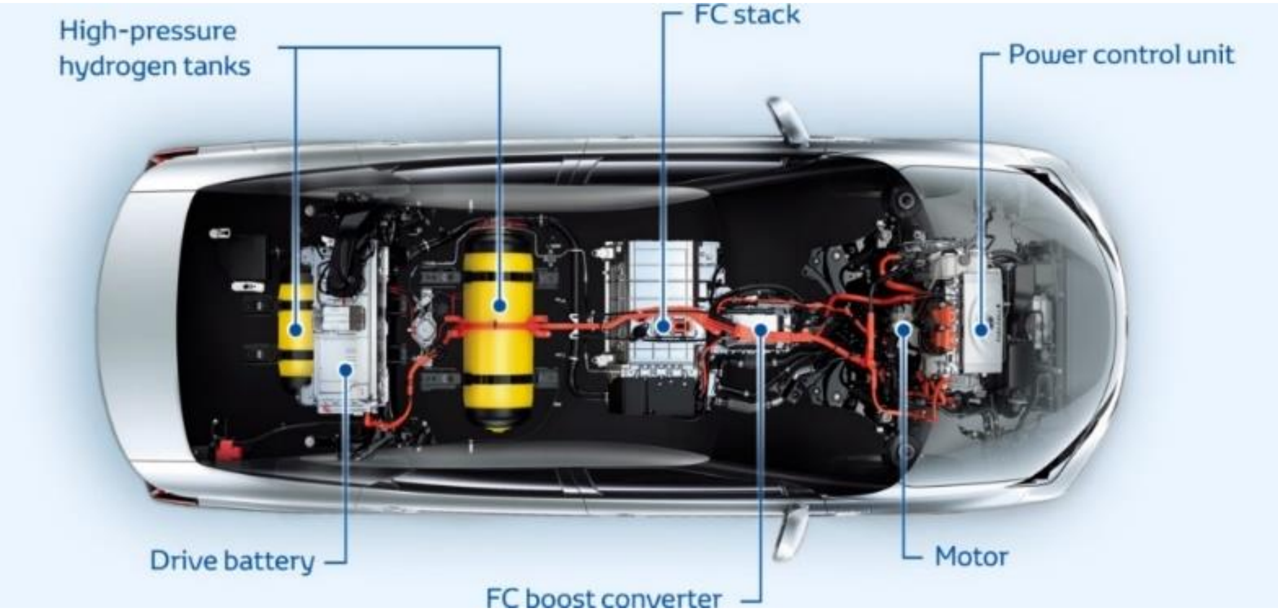
Theoretical efficiency $\eta = \Delta G / \Delta H =$ 83%

Practical efficiency: 50-60%

PEMFCs convert the chemical fuel (hydrogen) into electricity directly through electrochemical reactions with high efficiency.

No CO_2 emission or pollutants such as SO_x and NO_x.

Toyota Mirai



Power: 114 kW

Range: 312 mile

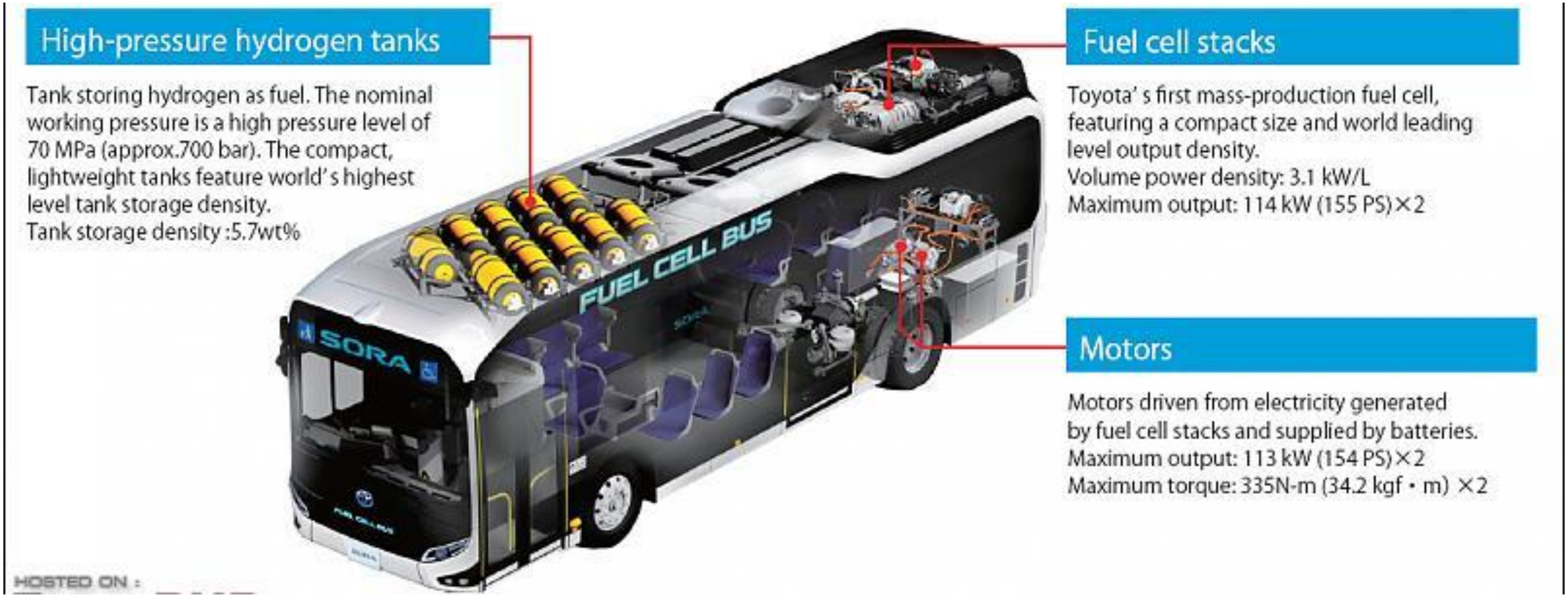
Refilling: 5 min

Hydrogen: 5 kg

Tanks + FC system: 140 kg

Price: ~£65,000

Toyota **Sora** fuel cell bus (SORA: an acronym for Sky, Ocean, River, Air)



High-pressure hydrogen tanks

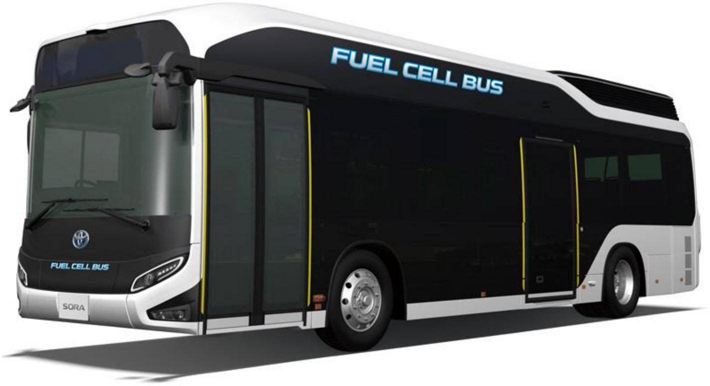
Tank storing hydrogen as fuel. The nominal working pressure is a high pressure level of 70 MPa (approx.700 bar). The compact, lightweight tanks feature world's highest level tank storage density.
Tank storage density :5.7wt%

Fuel cell stacks

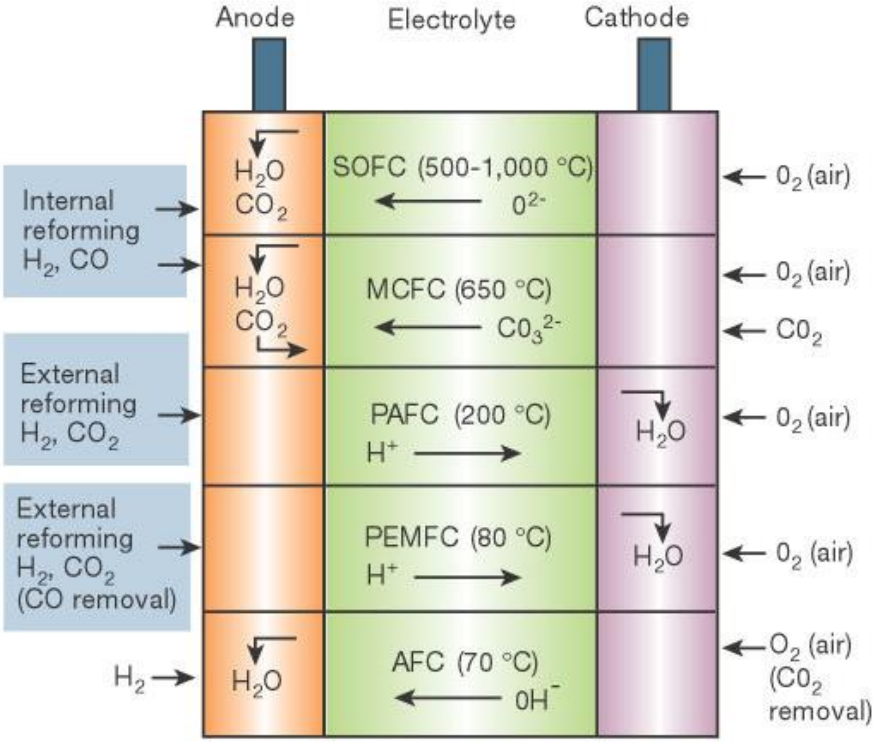
Toyota's first mass-production fuel cell, featuring a compact size and world leading level output density.
Volume power density: 3.1 kW/L
Maximum output: 114 kW (155 PS)×2

Motors

Motors driven from electricity generated by fuel cell stacks and supplied by batteries.
Maximum output: 113 kW (154 PS)×2
Maximum torque: 335N-m (34.2 kgf・m) ×2



Types of fuel cells:



Proton exchange membrane fuel cell (PEMFC)

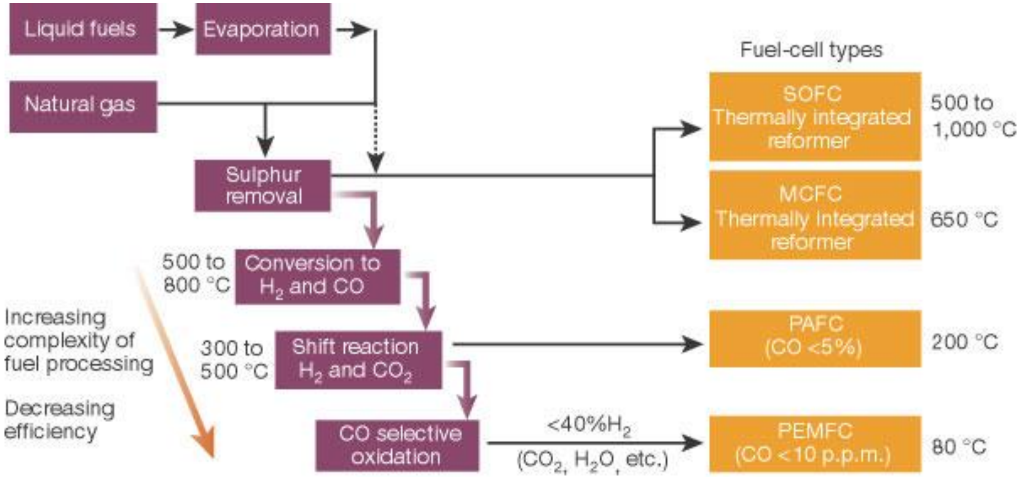
Direct Methanol fuel cell (DMFC)

Alkaline fuel cell (AFC)

Phosphoric acid fuel cell (PAFC)

Molten-carbonate fuel cell (MCFC)

Solid-oxide fuel cell (SOFC)



Nature 2001, 414, 345-352

PEMFCs

Advantages:

- High energy conversion efficiency
- Zero emissions or pollution
- Short refilling period (3-5 min)
- Long travel range

Disadvantages:

- Hydrogen generation, transport and storage
- Lack of hydrogen infrastructure (refilling stations)
- High costs
- Safety

Supercapacitors

Definition of capacitance

$$C = \frac{Q}{U} = \frac{\varepsilon_0 \varepsilon_r A}{d}$$

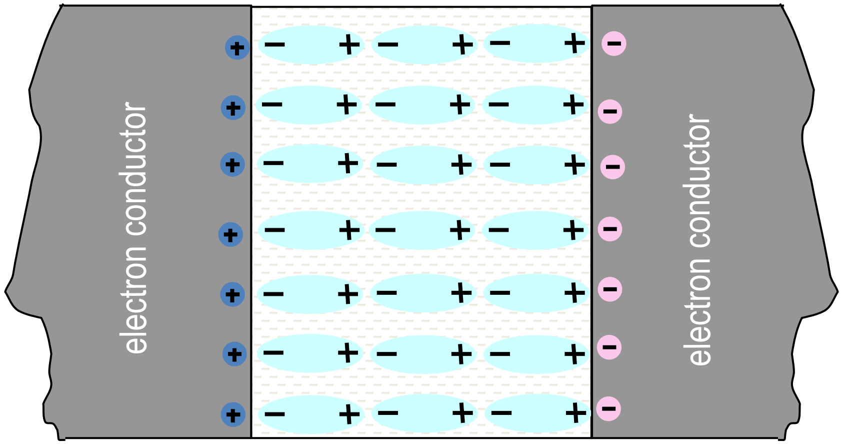
C: Capacitance; Q: Charge; U: Cell voltage

ε_r: Dielectric constant (relative permittivity)

ε_0: Vacuum permittivity (8.854×10^{-12} F/m)

A: Area of the interface between electrode and dielectric (or electrolyte)

d: Separation distance between electrodes

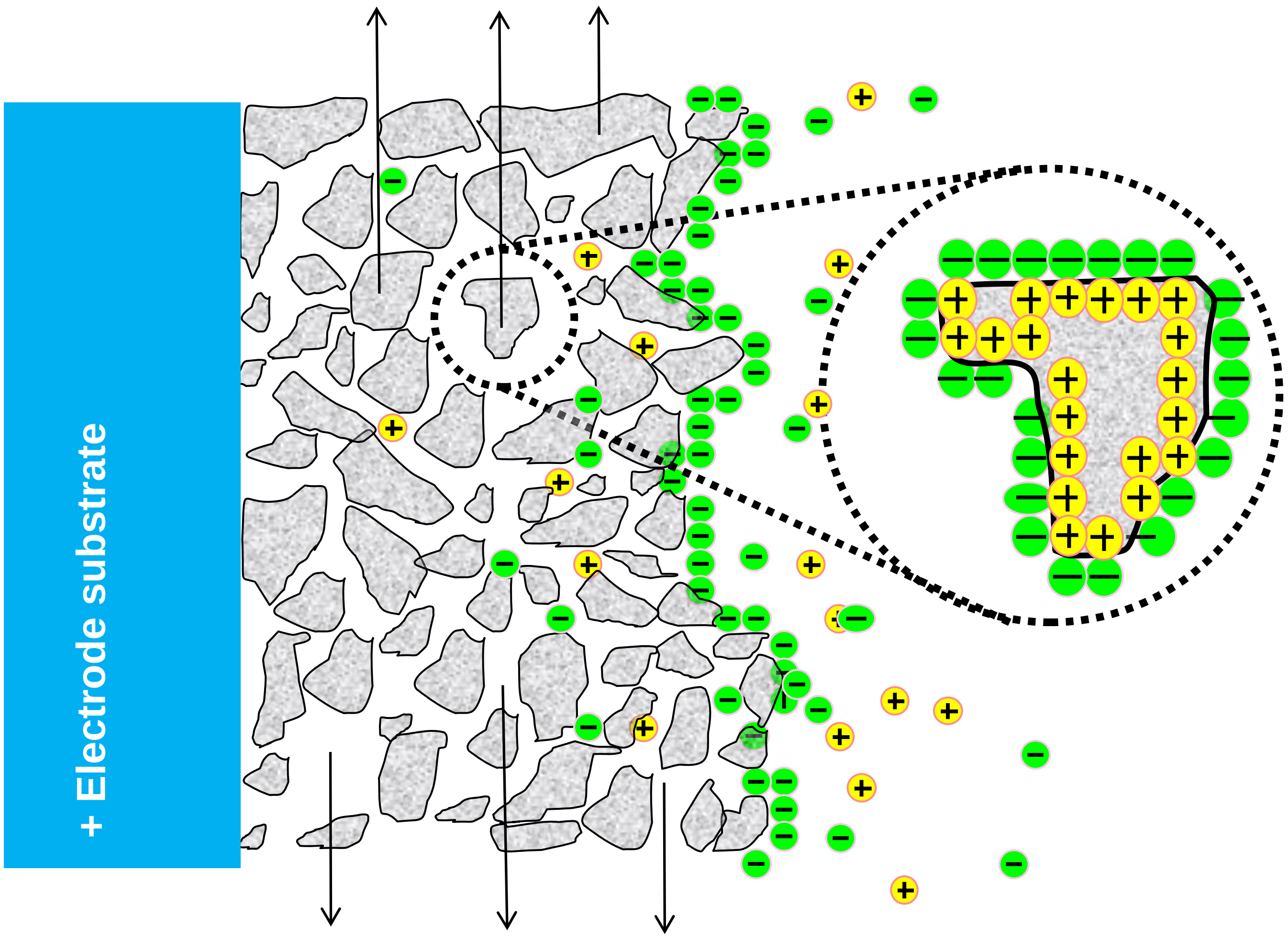


Dielectric capacitor

Supercapacitors with Double Layer Capacitance

Active electrode material
(Porous, high surface area activated carbon particles)

$$C = \frac{Q}{U} = \frac{\varepsilon_0 \varepsilon_r A}{d}$$



Electrolyte between particles and pores

The energy stored in a capacitor is given by:

$$E = \frac{CU^2}{2}$$

E = Energy
C = Capacitance
U = Voltage

Supercapacitors have very low specific energy.

Voltage: 3.0 V   Capacitance: 5000 F   Mass: 2,000 g

$E = CU^2/2 = 5000*3^2/2$

$= 22.5$ kJ $= 6.25$ Wh

Specific energy

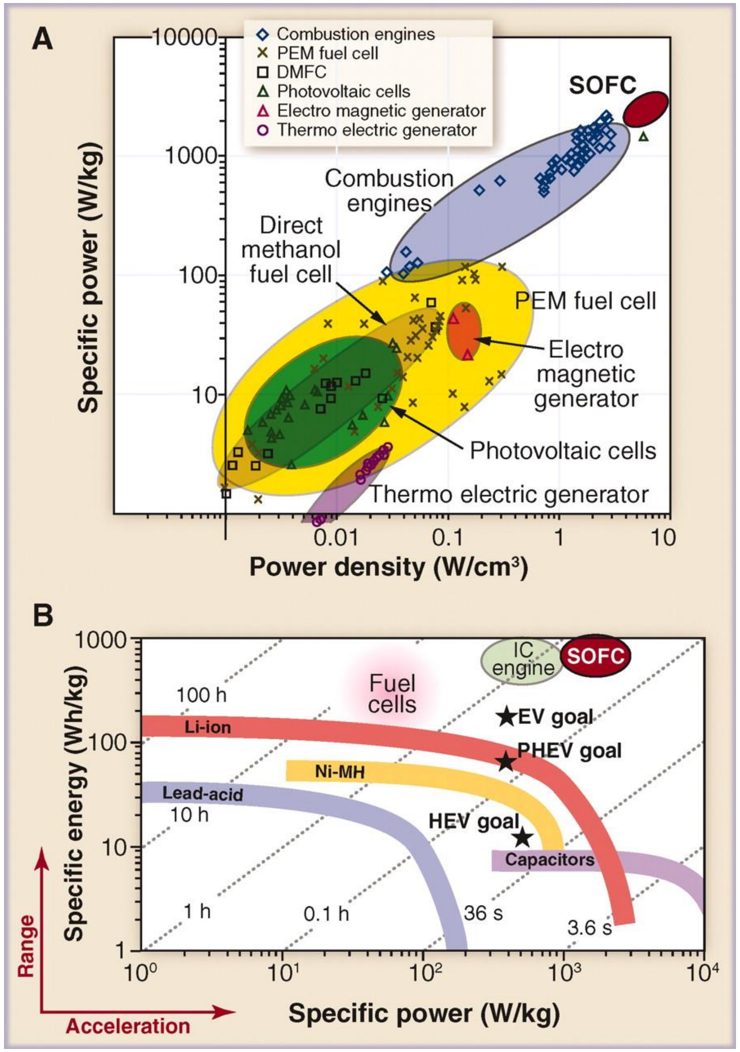
= 6.25 Wh / 2 kg

= 3.125 Wh/kg.

Advantages	Virtually unlimited cycle life; can be cycled millions of time
	High specific power; low resistance enables high load currents
	Charges in seconds; no end-of-charge termination required
	Simple charging; draws only what it needs; not subject to overcharge
	Safe; forgiving if abused
	Excellent low-temperature charge and discharge performance
Limitations	Low specific energy(1-10 Wh/Kg).
	Linear discharge voltage prevents using the full energy spectrum
	High self-discharge; higher than most batteries
	Low cell voltage; requires serial connections with voltage balancing
	High cost per watt

http://batteryuniversity.com/learn/article/whats_the_role_of_the_supercapacitor

https://www.mouser.co.uk/Maxwell-Technologies/Passive-Components/Capacitors/Supercapacitors-Ultracapacitors/_/N-5x76s?P=1z0ixuiZ1yfqekj



Science, 2011, 334, 935-939

(A) Comparison of specific power of various energy conversion devices as a function of power density.
(B) Ragone plot (specific energy versus specific power) for various energy devices.

Fuel	Energy by mass (Wh/kg)
Diesel	**12,700**
Gasoline	**12,200**
Ethanol	7,800
Black coal (solid)	6,600
Wood (average)	2,300
Li-ion battery	**250**
NiMH battery	**120**
Lead acid battery	**40**
Supercapacitor	**5**

http://batteryuniversity.com/learn/article/net_calorific_value

Combustion engine and gas turbine offer much higher power and energy density than batteries and supercapacitors.

Case study: designing future propulsion systems for transport

Key points:

Supercapacitor: high specific power but specific energy is too low. Cost is too high. Not suitable for vehicle propulsion systems.

Lead acid batteries: low specific energy. Long charging period. It is still commonly used for SLI applications in cars due to relatively low costs.

Lithium ion batteries: High specific energy. Cost is high. **The state-of-the-art battery system for vehicle propulsion systems**. Further increase in specific energy and decrease in cost are needed.

Hydrogen fuel cell: Requiring construction of new hydrogen filling stations. Challenges in hydrogen generation and storage.