Universidad del País Vasco
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Challenges and perspective in Materials for Energy Storage and Conversion Systems

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ESMolNa European School on Molecular Nanoscience

ESAM European School on Advanced Materials

W2dm Workshop on 2D Materials

19th European School on Molecular Nanoscience (ESMolNa 2026)

3rd European School on Advanced Materials (ESAM 2026)

12th Workshop on 2D Materials (W2DM 2026)

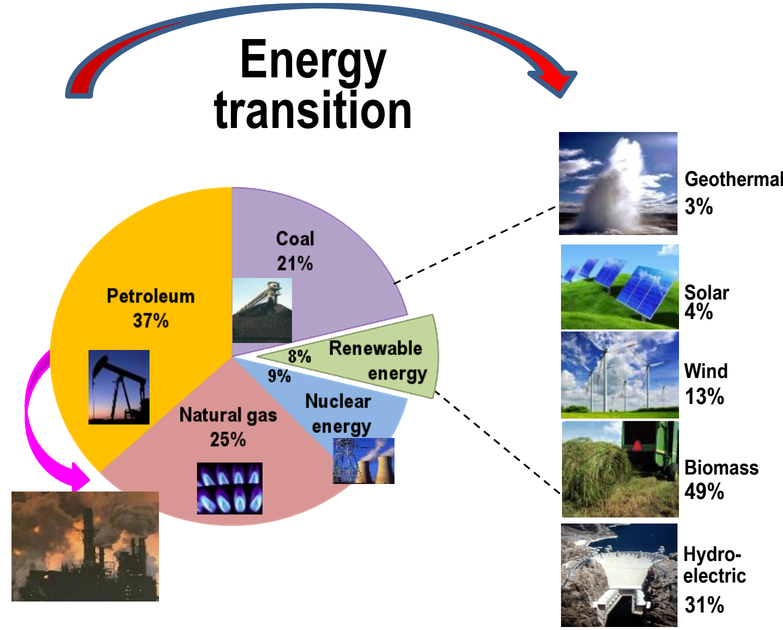
17th - 22nd May 2026 - Gandia (Valencia,Spain)

Outline

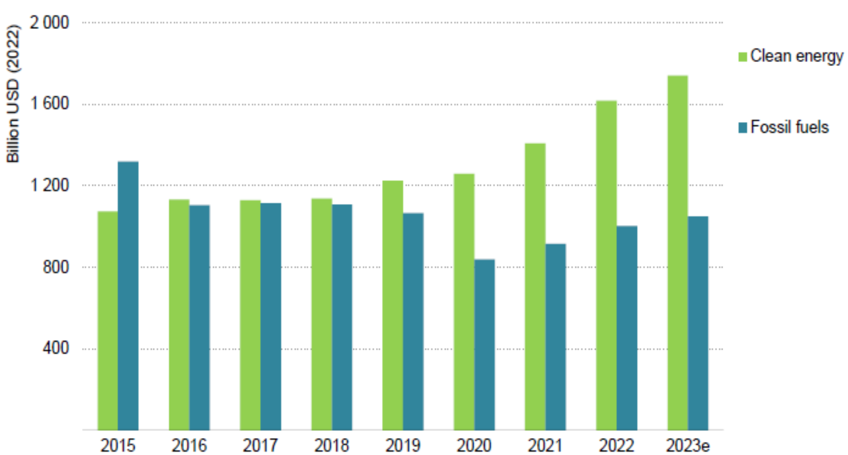
- Introduction
- Materials for Batteries
  - Electromobility
  - Stationary energy storage
- Materials for supercapacitors
  - Double layer capacitors
  - Pseudocapacitors
  - Hybrids
- Materials for Full Cells
  - Hydrogen as energetic vector
  - Electrolyzers
  - Mobility
- Summary and conclusions

(14 TW) → **(28 TW)**

http://americanenergyindependence.com/energychallenge.aspx

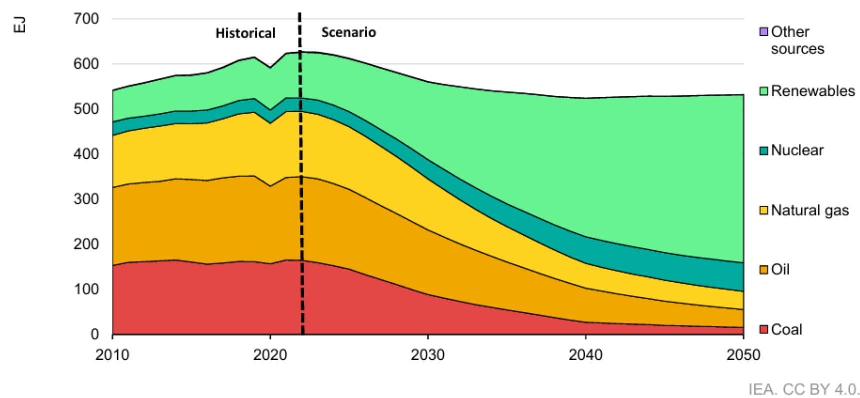


Global energy investment in clean energy and in fossil fuels 2015-2023

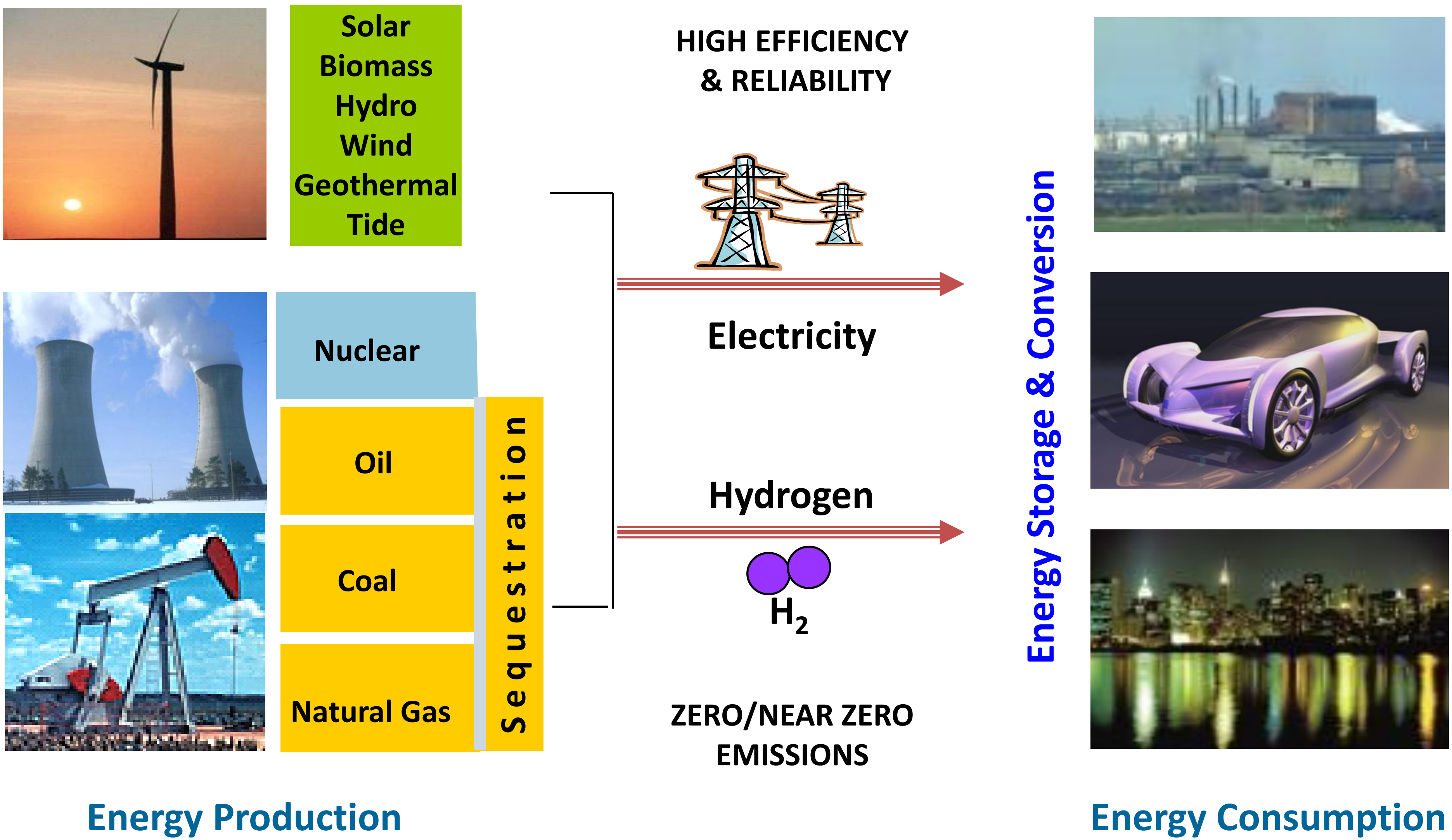


Estimated values for 2023 , IEA2023

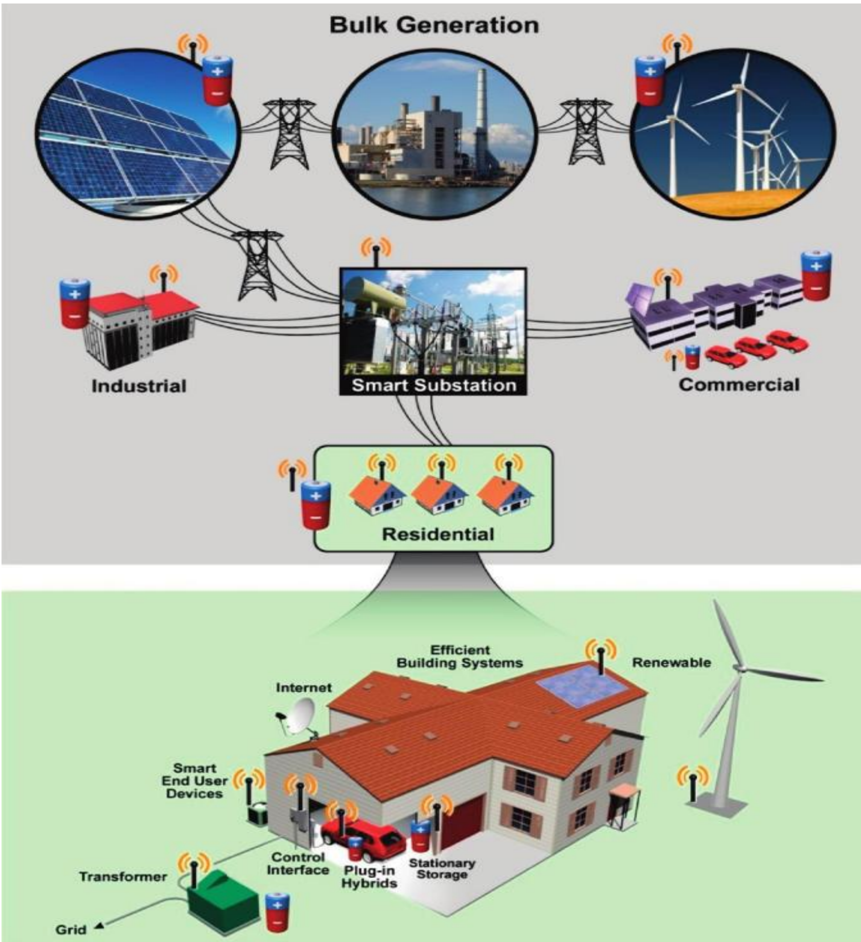
Global total primary energy supply in the NZE Scenario

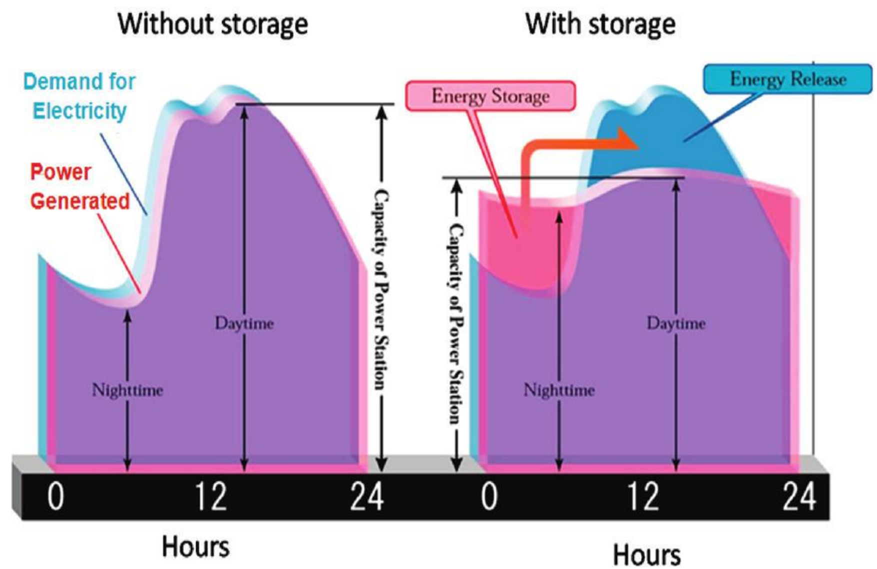


Renewables and nuclear displace most fossil fuel use in the NZE Scenario, with the share of fossil fuels plunging from almost 80% in 2021 to less than 20% in 2050.


Solar
Biomass
Hydro
Wind
Geothermal
Tide
Nuclear
Oil
Coal
Natural Gas
Sequestration
HIGH EFFICIENCY & RELIABILITY
Electricity
Hydrogen
H_2
ZERO/NEAR ZERO EMISSIONS
Energy Storage & Conversion
Energy Production
Energy Consumption

Energy storage for generation, transmission and distribution





Storage is critical

- Frequency regulation and load following.
- Cold start services.
- Contingency reserves.
- Energy services that shift generation from peak to off-peak periods.

Batteries constitute the critical part of the available energy storage systems.

Chem. Rev. 2011, 111, 3577–3613

Mid-term needs in Energy Storage

Automobiles

1.10^{9} cars 10% electric

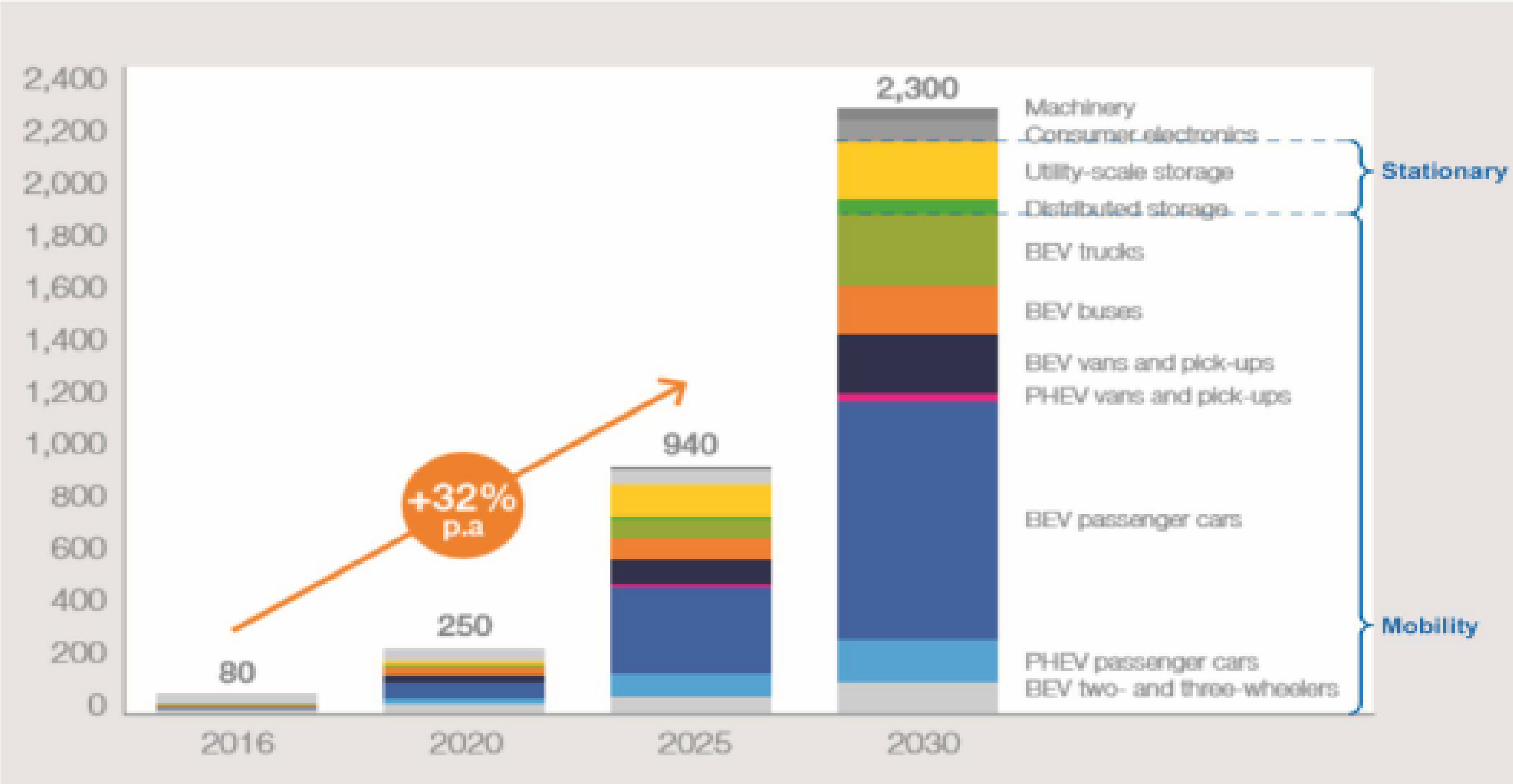
➔ 200.10^{6} tons batteries

Load-leveling

World electricity production
= 2.10^{13} kWh 10% stored/d

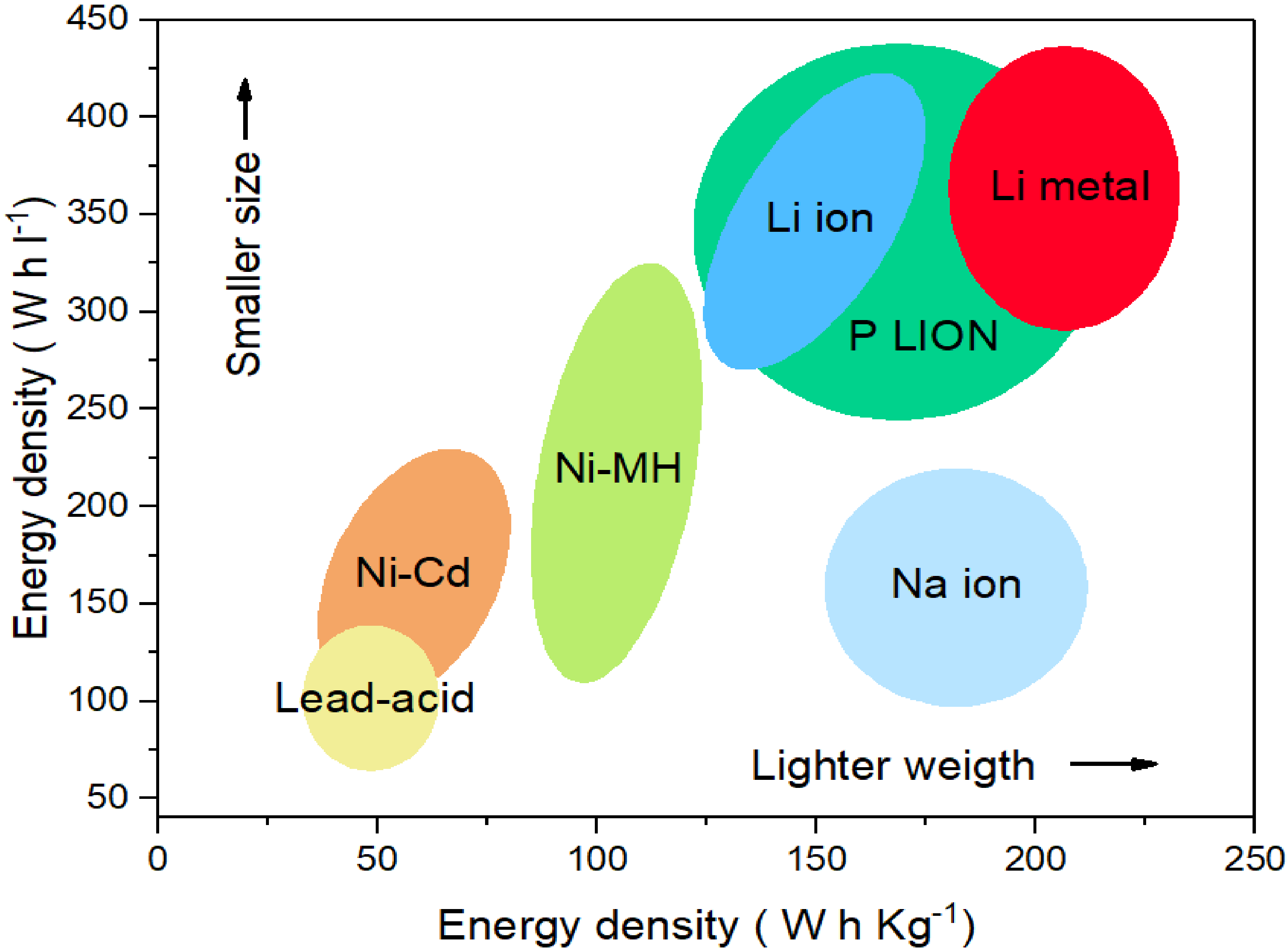
➔ 10^{9} tons batteries

Battery demand (GWh/yr)



Annual battery demand:
Electric mobility segments, stationary battery storage, consumer electronics, and machinery (GWh/yr)

Battery Technologies



Comparison of the different battery technologies in terms of volumetric and gravimetric energy density.

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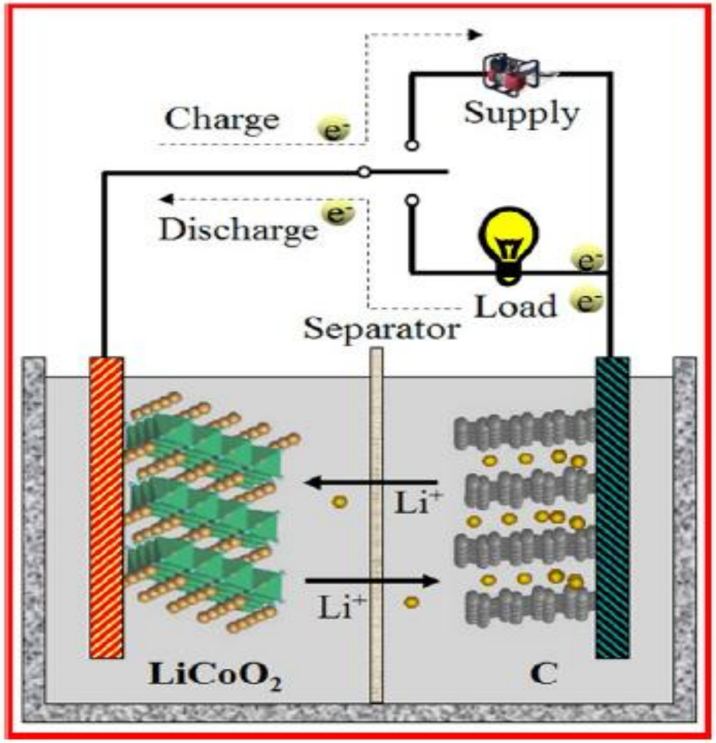
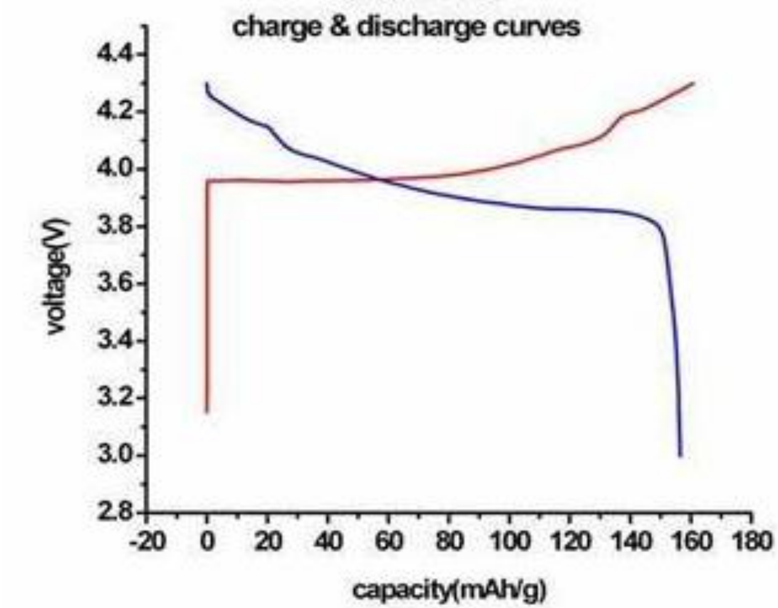
Working of the Li-ion Battery





Charge/discharge of $LiCoO_2$ vs Li/Li^+.

Charging Reaction:

- **Cathode**: $Li_xCoO_2 \rightarrow Li_{x-y}CoO_2 + y \cdot Li^+ + y \cdot e^-$
- **Anode**: $yLi^+ + ye^- + C_6Li_{1-x} \rightarrow C_6Li_{1-(x+y)}$

Discharge Reaction:

- **Anode**: $C_6Li \rightarrow xLi^+ + x \cdot e- + C_6Li_{1-x}$
- **Cathode**: $xLi^+ + x \cdot e^- + CoO_2 \rightarrow Li_xCoO_2$

Cell Reaction: $LiC_6 + CoO_2 \xrightarrow{\text{discharge}} C_6 + LiCoO_2$ E = 3.7 V at 25°C

Cell voltage: difference in voltage of the cathode and the voltage of the anode.

Basic performance parameters of a battery cell

- **Capacity**: the amount of Li that is stored in each electrode

Theoretical specific capacity:

$$Q_t\ (mAh\ g^{-1}) = nF\ /3.6M$$

n is the number of transferred electrons , ***F*** is the Faraday constant (96485 C mol^{-1}), ***M*** is the molecular mass of the active material.

- **Energy density**: Capacity x voltage of the cell.

Theoretical specific energy:

$$E_t\ (kJ/kg) = (nE/M_t)\ F \qquad E_t\ (Wh/kg) = 26{,}805\ (nE/M_t)$$

n is the number of transferred electrons per mol, ***F*** is the Faraday constant, ***E*** is the average voltage (V) and M_t (g/mol) the sum of the molecular weights of all the reactants. (Watt is 1Joule per second, 1J=1Cx1V and 1Wh is 3,6 kJ)

- **Power density** *(W/kg)*

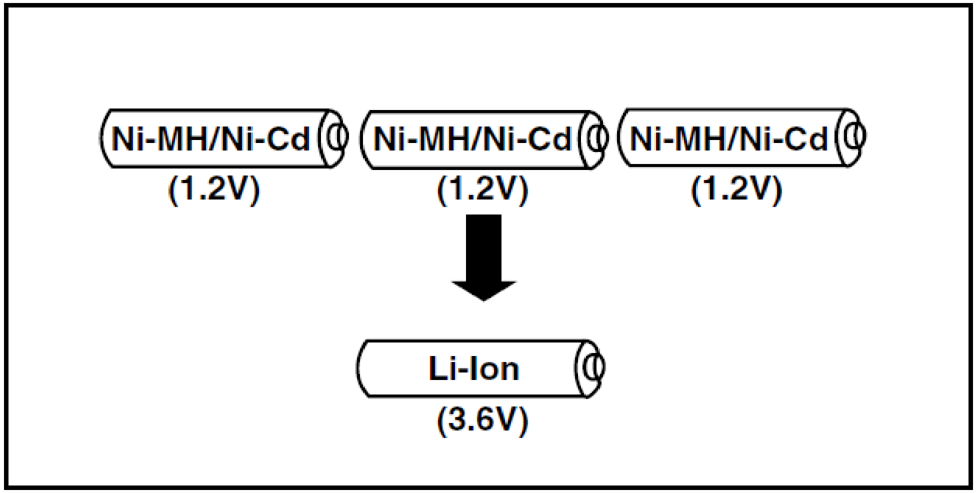
How quickly the Li is transferred from one electrode to the other.

Energy Density of a battery cell

➢ Volumetric energy density : Wh/L

Energy stored in a specific volume of the cell.

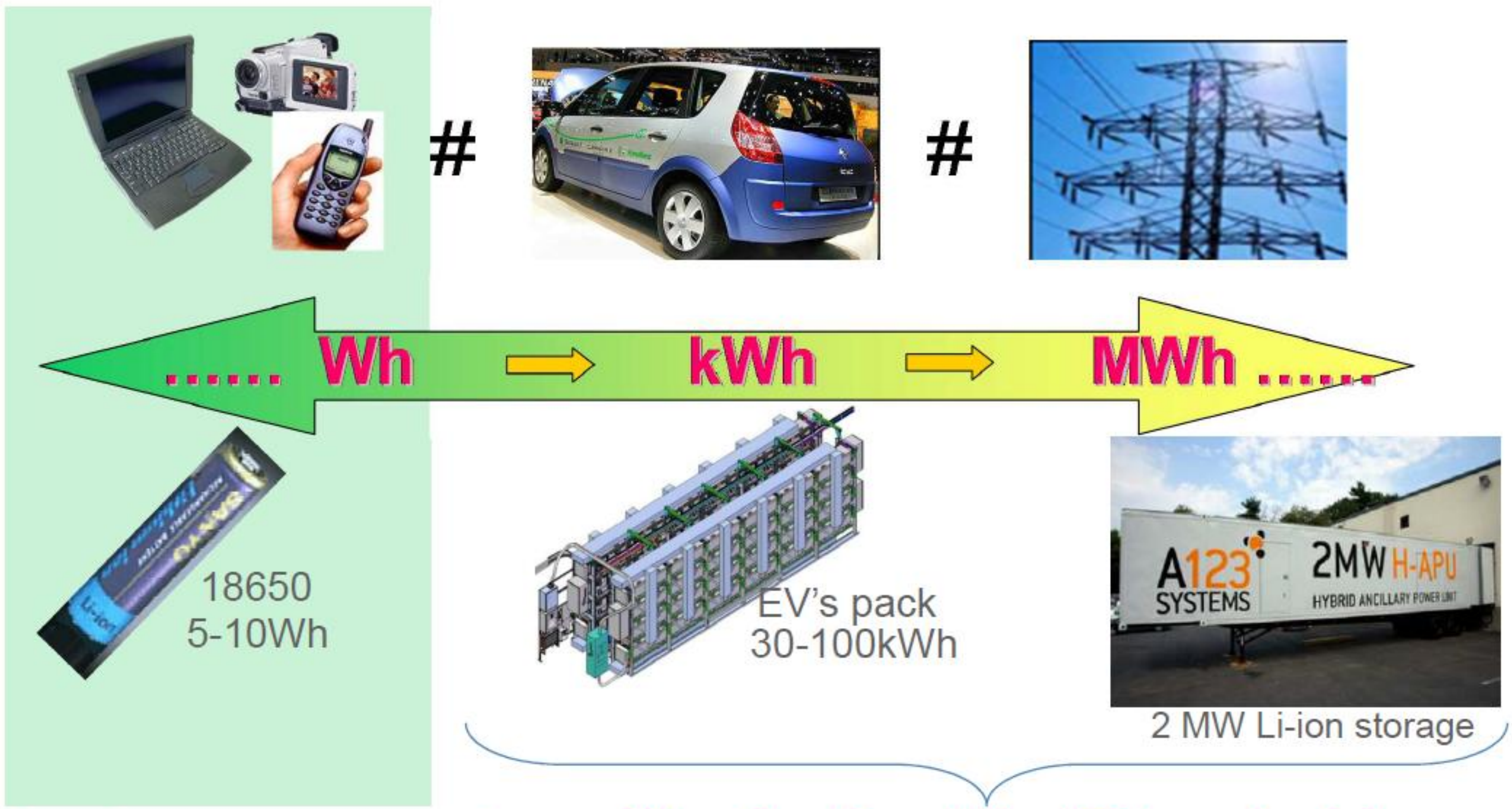
More dominant or important where space is the limit : Eg. Cell phones, laptops, cars etc.



➢ Gravimetric energy density : Wh/kg

Energy stored in a specific amount of the material in the cell.

Li-ion Technology

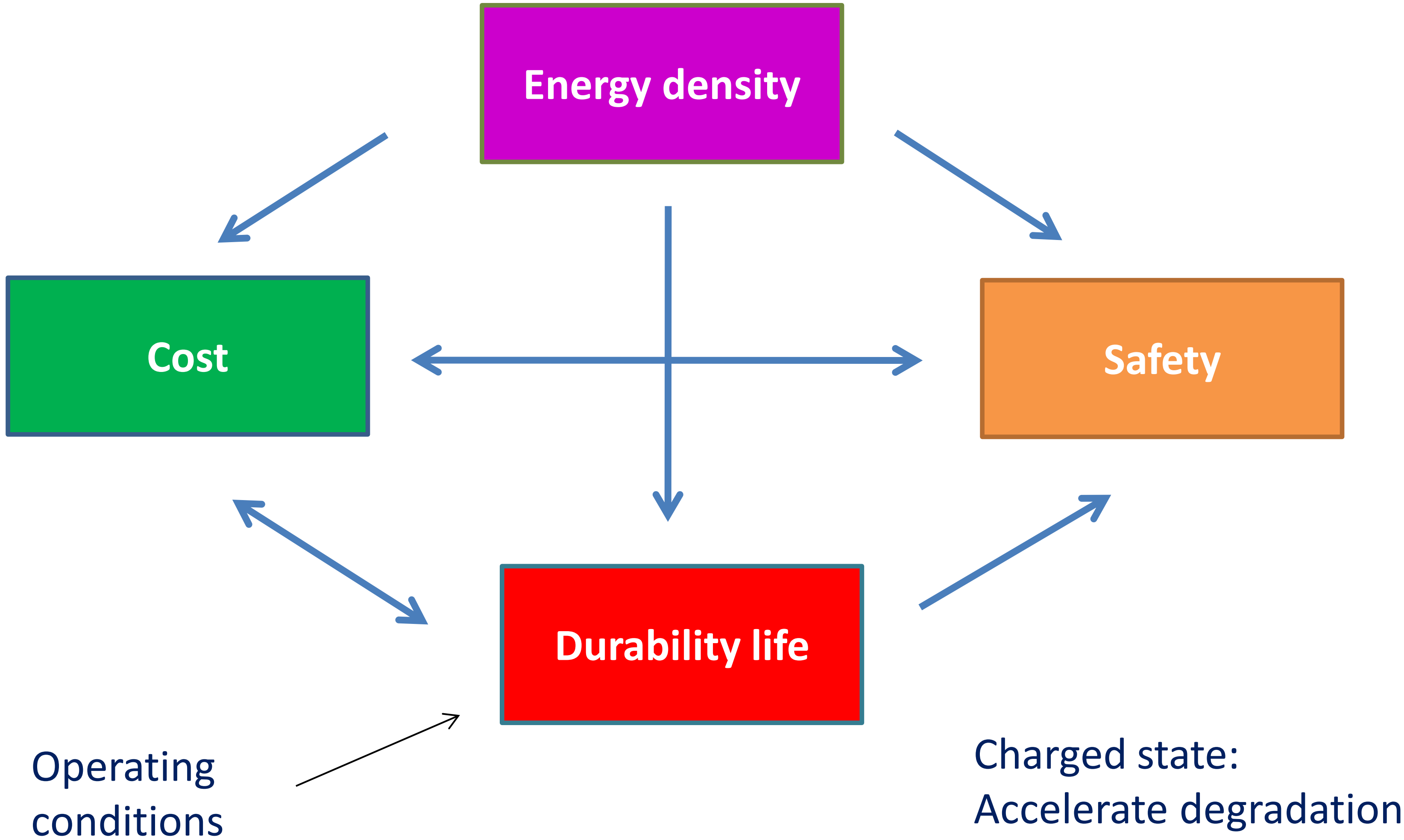


Li-ion has conquered the portable market ..

What's about the EV and grid applications markets ???

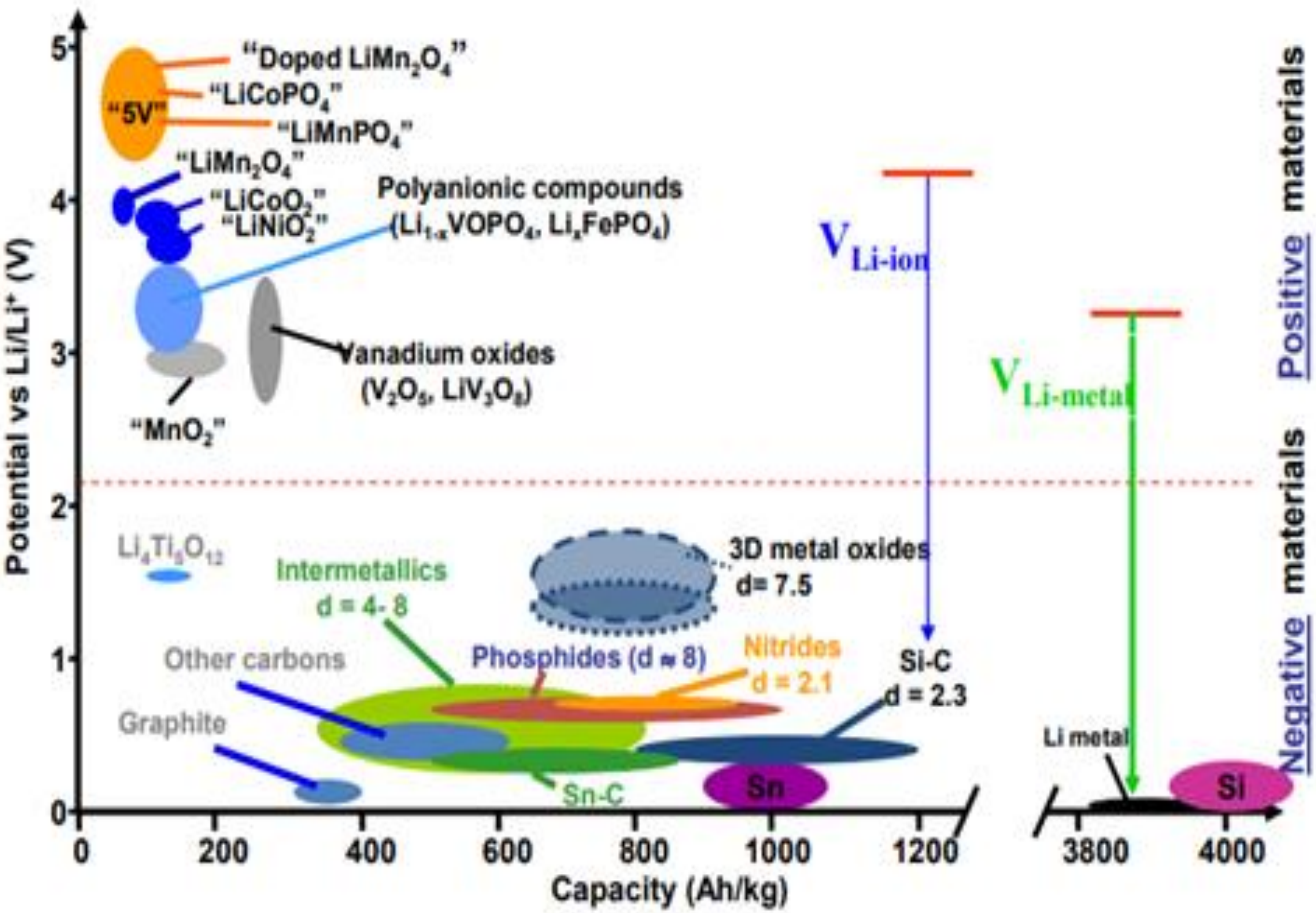
Is the use of Li-ion Batteries necessary or appropriate for stationary energy storage (MWh-GWh)?

Energy Storage for Batteries



None of the presently-studied chemistries appear to satisfy all four criteria

Materials for Li-ion Batteries



TESLA MOTORS: NMC, NCA, Graphite

BOLLORE: LFP/ Polymer electrolyte/Li

NISSAN LEAF: LMO-NMC, Graphite

BYD: LFP, Graphite

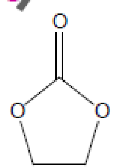
Electrolyte used in Lithium Ion Batteries

mixture of solvent(s) and salt

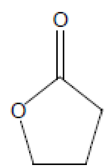
solvent

dielectric constant ε ↗

cyclic carbonates



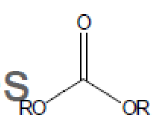
cyclic esters



+

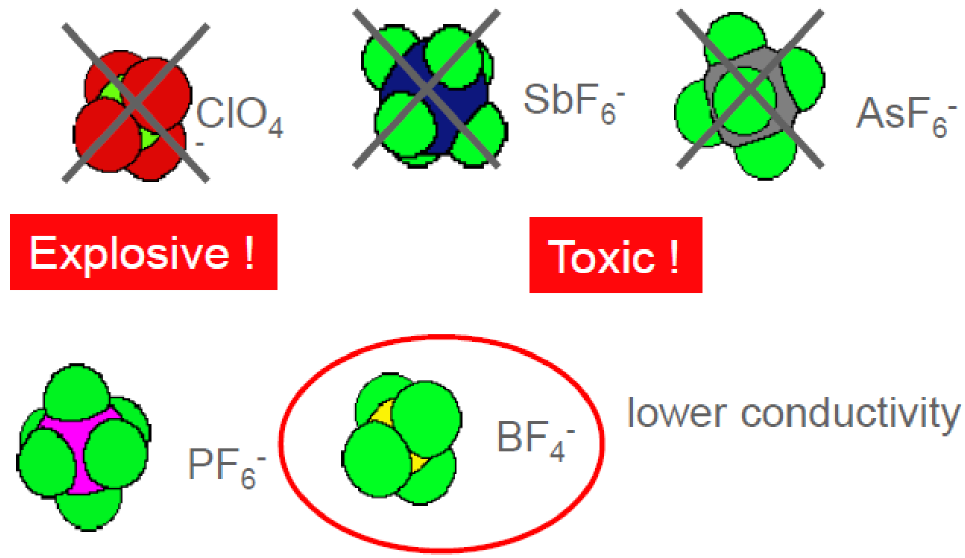
viscosity η ↘

linear carbonates



ethers

salt



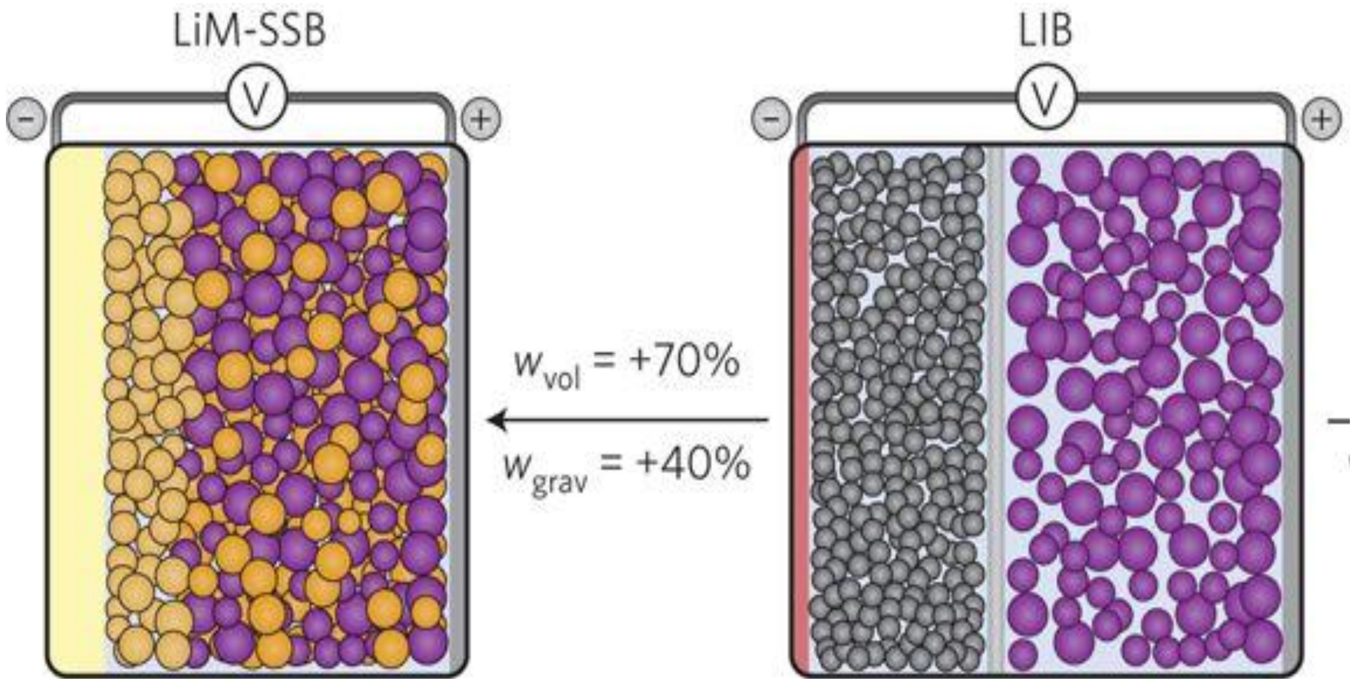
- **Most Organic solvents decompose above 4.3V.**
- **Cost and flammability of the organic electrolytes remain a problem.**

Li-ion Batteries generations

Generation	1	2		3		4			5
		2a	2b	3a	3b	4a	4b	4c	
Type	Current	Current	State-of-the-Art	Advanced Li-ion HC	Advanced Li-ion HV	Solid State			Beyond Li-ion
Expected Commercialisation	Commercialised	Commercialised		2020	2025	>2025			
Cathode	• NMC/NCA • LFP • LMO	• NMC111	• NMC424 • NMC523	• NMC622 • NMC811 • NMC910	• HE NMC • Li-rich NMC • HVS	• NMC	• NMC	• HE NMC	• O_2 • S
Anode	• Modified Graphite • $Li_4Ti_5O_{12}$	Modified Graphite	Modified Graphite	Carbon (Graphite)+Si (5-10%)	Silicon/Carbon (C/Si)	Silicon/Carbon (C/Si)	Li metal		Li metal
Electrolyte	• Organic • $LiPF_6$ salts				• Organic+ Additives	• Solid electrolyte – Polymer (+Additives) – Inorganic – Hybrid			
Separator	Porous Polymer Membranes								

- **M-O_2 currently at TRL2-3; expected performance and applications (still early to define accurately).**
- **The research in All Solid State Batteries is currently predominant.**

Advantage of Solid State Batteries



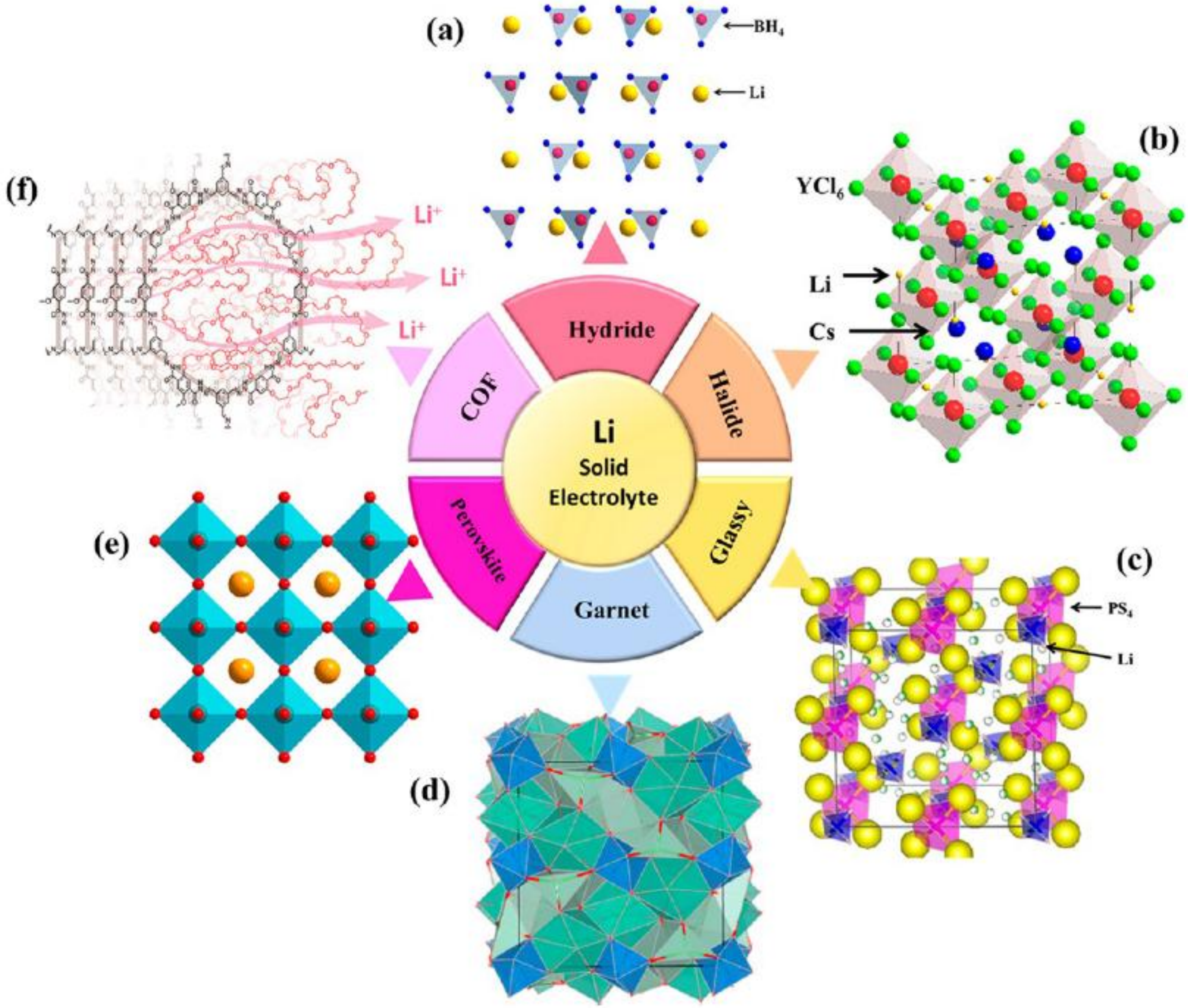
If Li metal can be used:

Volumetric energy density: w_{vol}=+70%
Gravimetric energy densities
w_{grav}=+40%

- ☑ Avoid or diminish the safety problems
- ☑ High thermal stability
- ☑ Wide electrochemical stability window
- ☑ Excellent mechanical properties.
- ☑ No dendrites formation

- ☒ Low ionic conductivity at RT

Solid Li-ion electrolytes

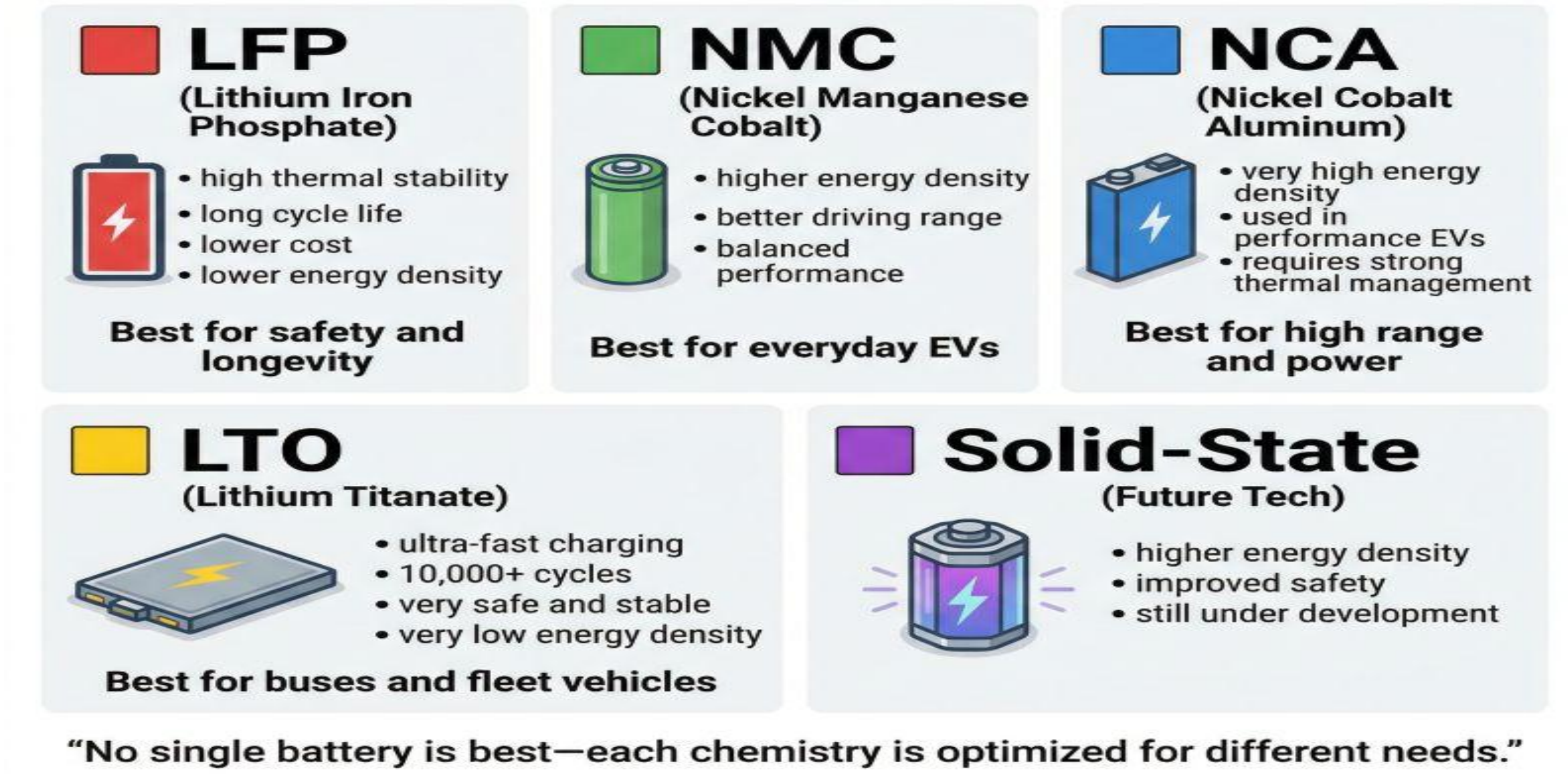


Covalent organic framework COF-PEOx (x=3,6,9)

Solid State Bateries

GOOD FAIR POOR	Polymer	Oxides	Sulfides	Halides
	PEO	*LLZO*	*Li_2S-nP_2S_3 Blends*	*Li_3YCl_6, Li_3InCl_6*
Material Phase	Amorphous	Crystalline	Crystalline or Glass	Crystalline
Ionic Conductivity				
Air Stability				
Stability *vs.* Li Anode				
Stability *vs.* High-V Cathode				
Easy of Manufacturing/ Processing Technique	**Roll-to-roll**	**Sintering**	**Roll-to-roll**	**Too early**
Stack Pressure Required	✓	✓	✓	✓
Companies	Hydro Québe, BOLLORÉ LOGISTICS, SEEO	ion Storage Systems, QuantumScape	TOYOTA, Polyplus transfection, SAMSUNG, Solid Power	None at this time

EV Battery Chemistry



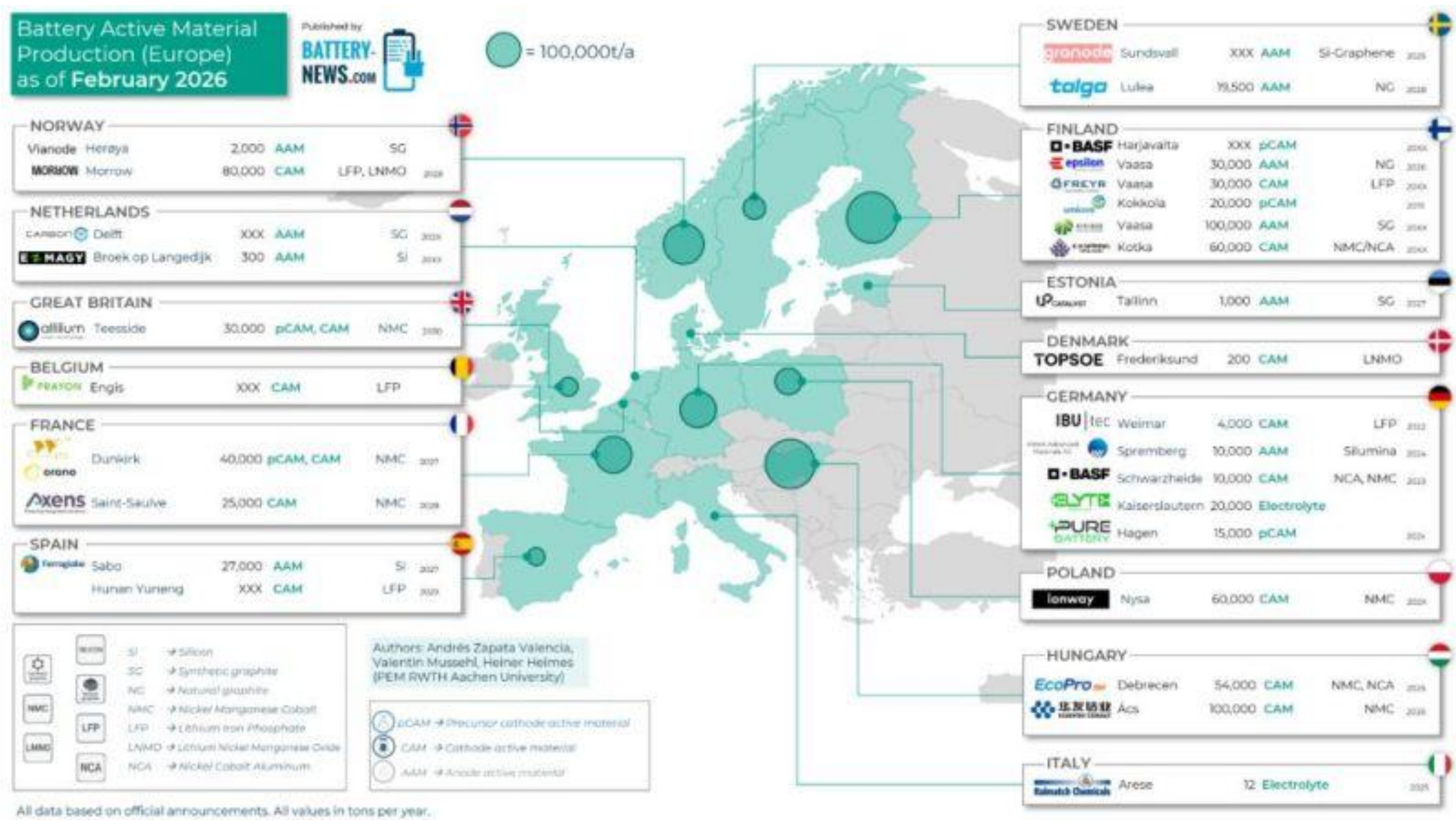
Energy density:

- Conventional Li-ion energy density ranges from 160 (LFP) to 275 Wh/kg (NMC)
- An increase to 400-500 Wh/kg is needed to reduce cost significantly.

Toxicity of materials:

- Companies are currently positioning themselves for the use of LFP as cathode material instead of NMC despite its cost in energy density.

Battery Active Materials Production (Europe 2026)



https://www.linkedin.com/posts/battery-news_battery-materials-supplychain-activity-7453543886930612224

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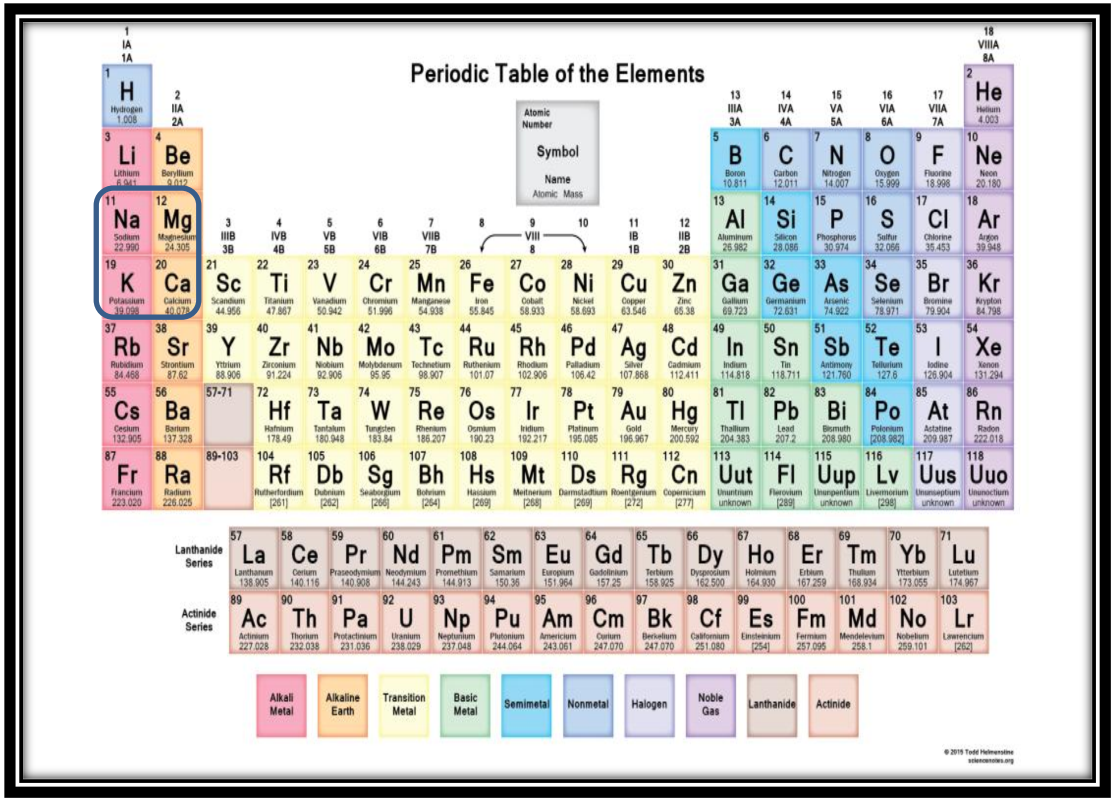
Let us look back for a while to look ahead

Battery concept based on different elements has been analyzed in the recent years



Magnesium (Mg), Calcium (Ca), Aluminum (Al) batteries show very slow progress with many difficulties to go to the market.

Vanadium redox flow batteries

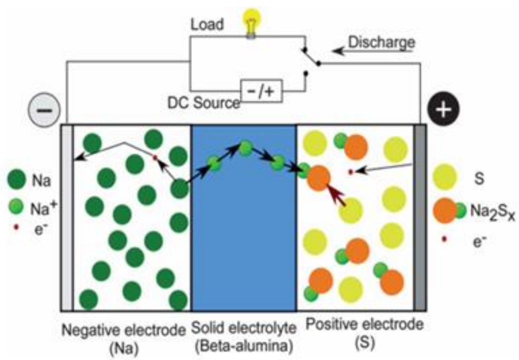
- Expensive ($ 300-500/kWh or higher) → too high for commercialization
- Excellent electrochemical reversibility **but** high cost and toxicity of vanadium.

> - **Large Energy Storage is a great challenge.**
> - **Na based systems seem to be the best alternative for stationary applications.**

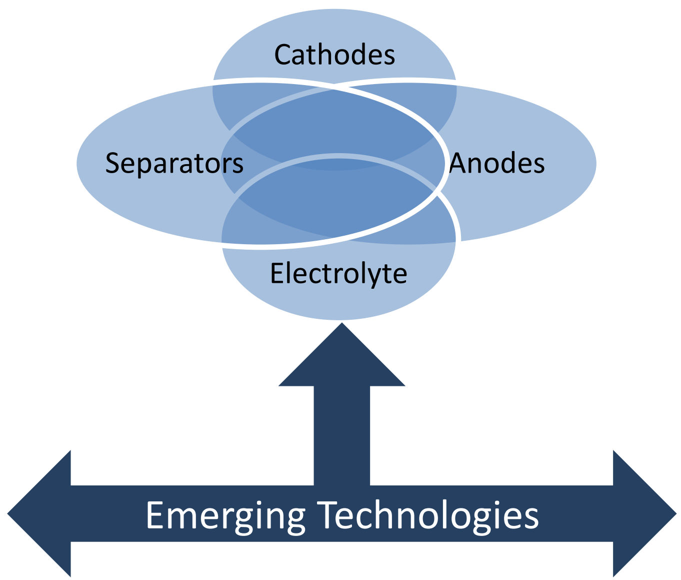
Na-Based batteries

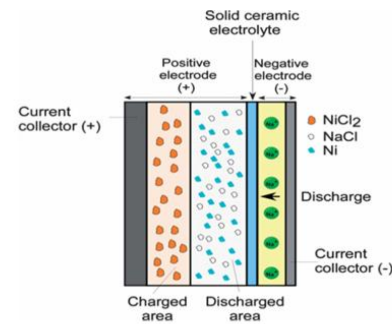
Sodium ion non aqueous → Sodium ion aqueous → Sodium sulfur HT → ZEBRA HT → Sodium Air

R&D/Demo | Demo | Commercial | R&D



Na-S HT





Zebra HT

Na ion non aq.

- Low Cost
- High Power
- High voltage among other Na systems

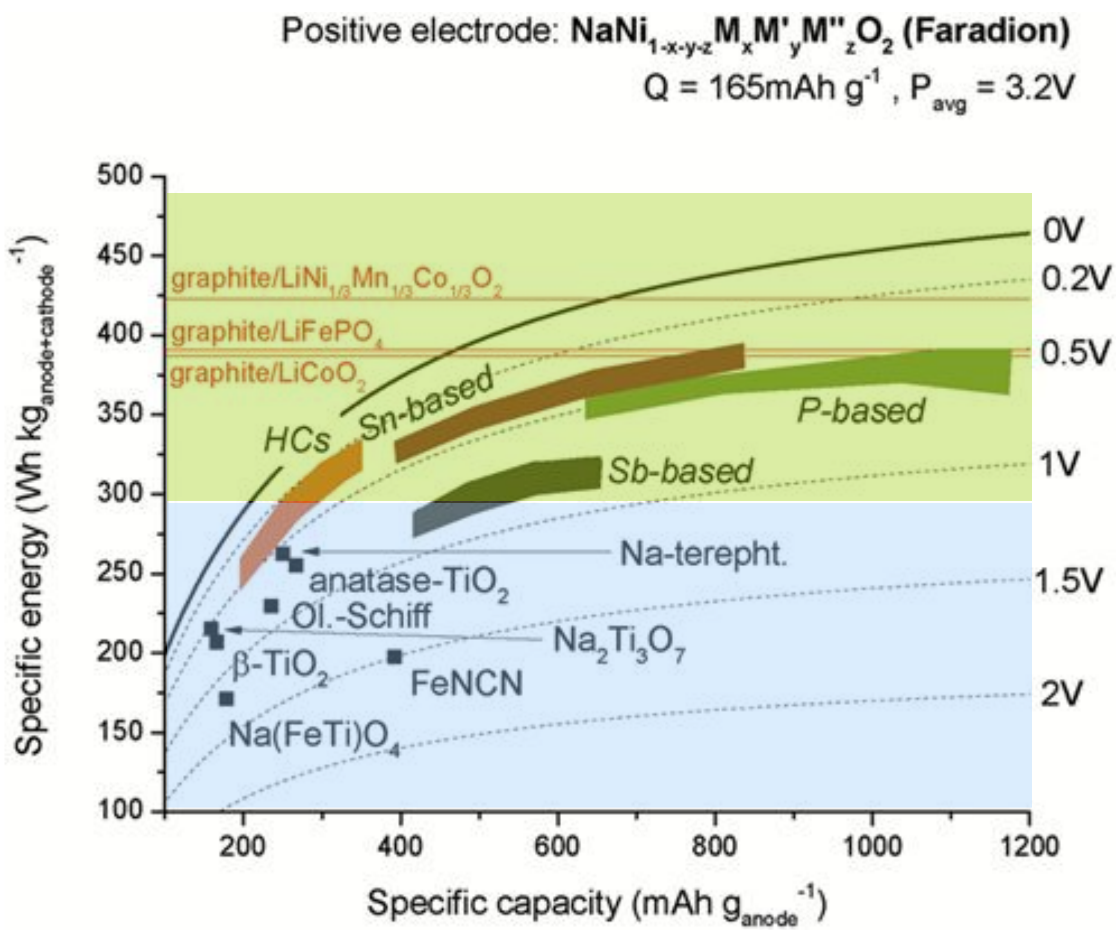
Low Temp Na - S

- Low Cost System
- Low Operating cost
- High Energy
- Safety
- Established Engineering

Scale Up of Materials For Prototypes !!!!

Anode materials for Na-ion batteries

Anode materials can be divided in 2 groups:



Energy density > 300 Wh·kg$^{-1}_{(anode+cathode)}$

- Carbons
- Alloys (Sn or P-based)

Energy density ≈ 250 Wh·kg$^{-1}_{(anode+cathode)}$

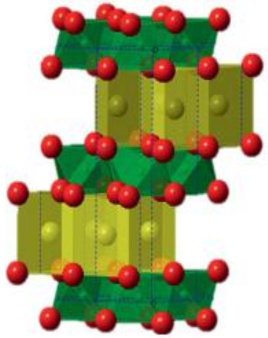
- Organic electrodes
- Oxide materials

T. Rojo et al, *Adv. Energy Mater.* **2017**, *7*, 1700463.

Na-ion battery cathodes

Sodium layered oxides

e.g. $Na_xT_MO_2$, etc.

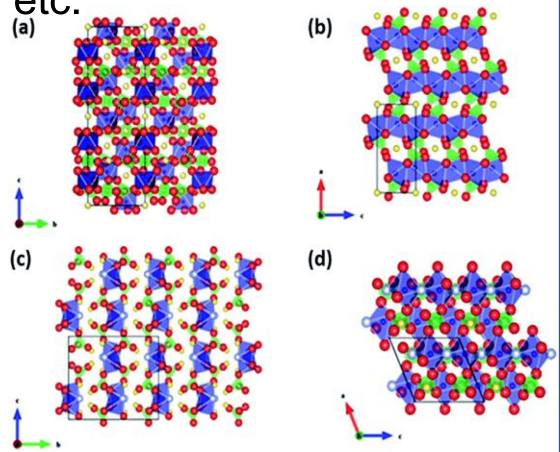


- High reversible capacities: ~200 $mAhg^{-1}$
- High specific energies: ~600 $Whkg^{-1}$
- High rate capability
- Facile technology transfer

- Generally highly hygroscopic
- Relatively low potentials: 2.8 – 2.9 V vs. Na^+/Na
- Poor cyclability (multiple phases and large internal expansion)

Polyanionic materials

e.g. NASICON, NaFP, etc.

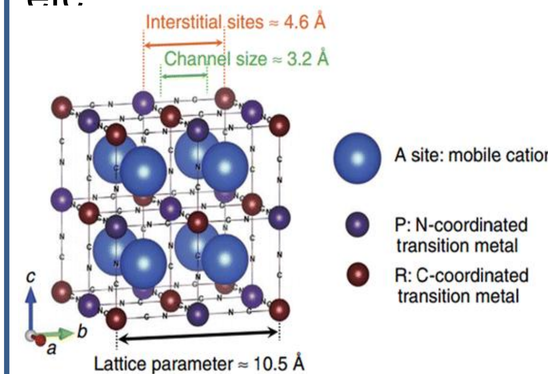


- Good thermal stability
- Not hygroscopic

- Relatively low reversible capacities: ~120 $mAhg^{-1}$
- Low specific energies: ~300-400 $Whkg^{-1}$
- Chemical preparation of olivine phases

Prussian blue

e.g. $Na_xT_MFe(CN)_6$, etc.

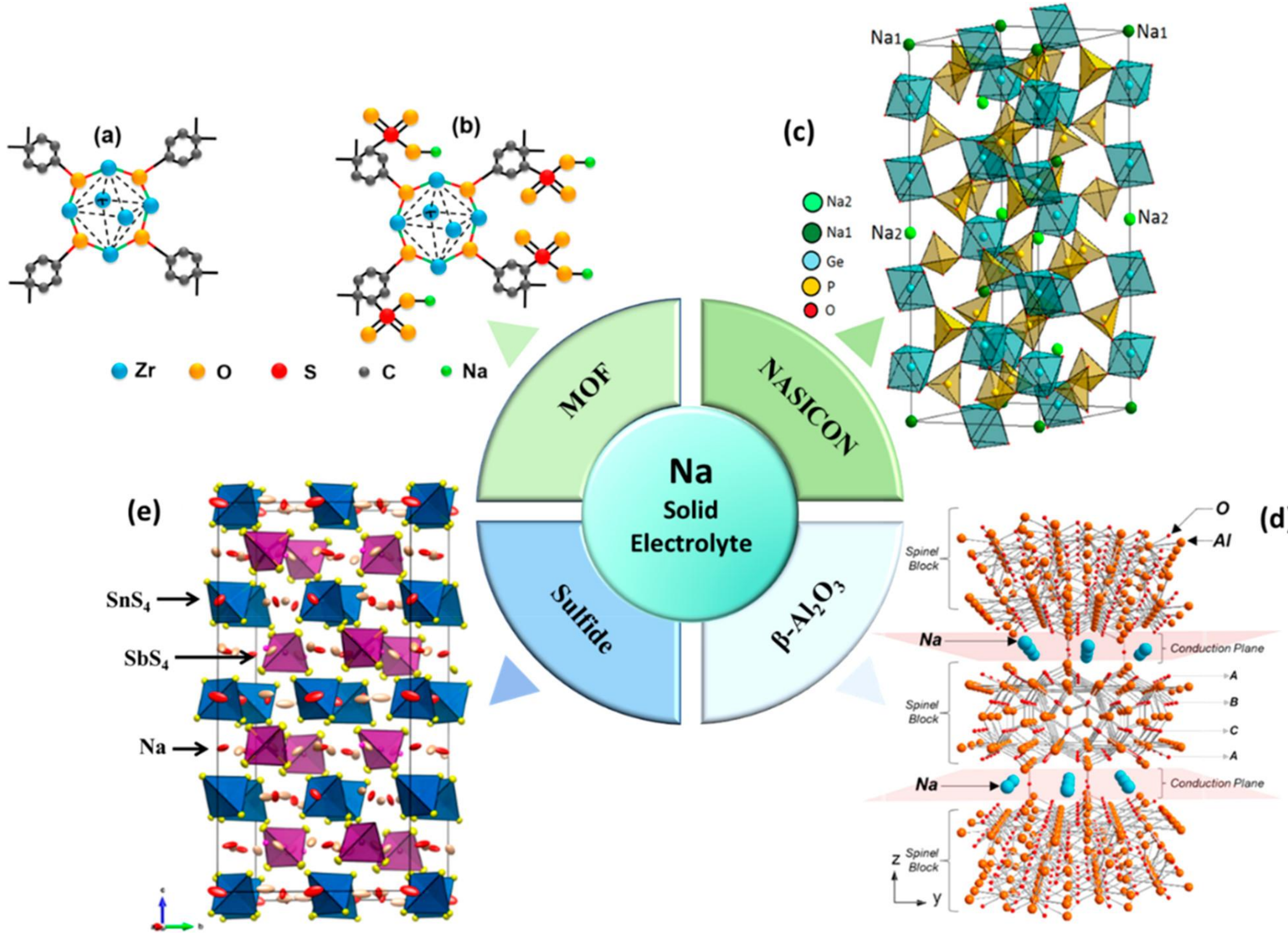


- Wide range of potentials
- High reversible capacity
- High energy densities: ~500-600 $Whkg^{-1}$
- Low synthesis temperatures

- High amount of conductive carbon needed
- Coulombic efficiency needs improvement

Jahn-Teller distortion present in all materials, most significant effect in 2D layered oxides

Structures of typical solid Na electrolytes.

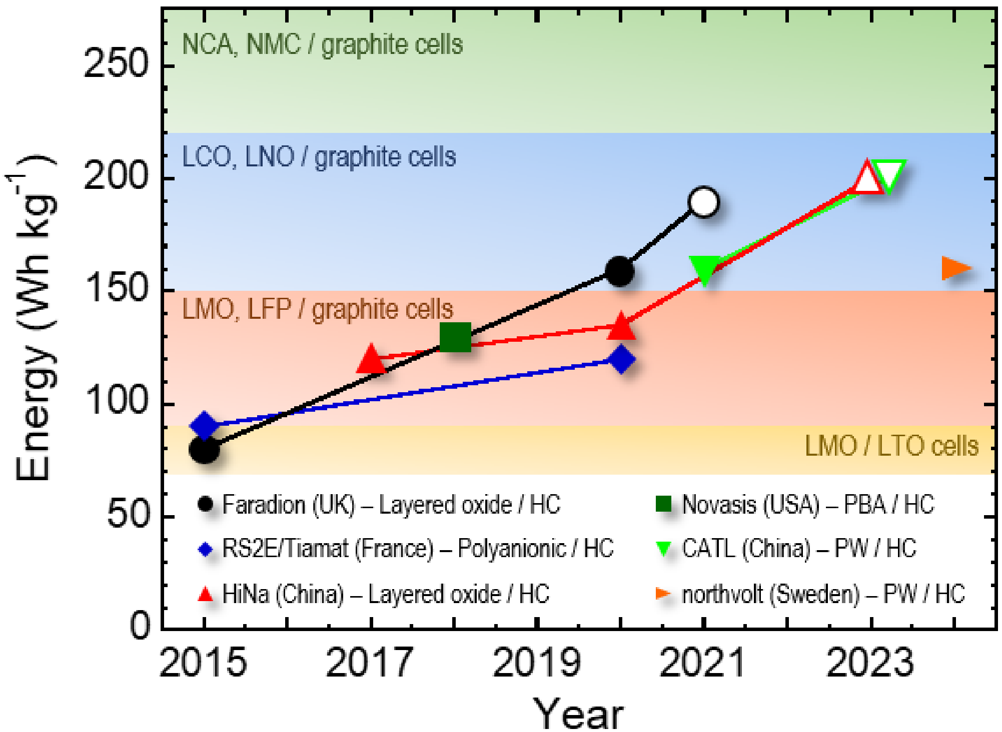


(a) Structural schematic of UIO-66 (U Oslo) MOF and
(b) structure of UIOSNa (UIO-66 with −SO3Na functional groups grafted).
(c) Structure of NASICON (NaGe2(PO4)3).
(d) Structure of Na-β-alumina with Na+ located in the conduction plane between densely packed spinel-like alumina blocks
(e) Structure of Na11Sn2SbS12 along [100].

DOI: (10.1021/acs.chemmater.2c01475)

Sodium ion batteries: prototype and commercial cells

Commercially available nonaqueous NIBs



- CATL, BYD and CTG will put this technology on the market in 2026
- Altris (Sweden) also developing NIBs of more than 100 Wh kg^{-1}

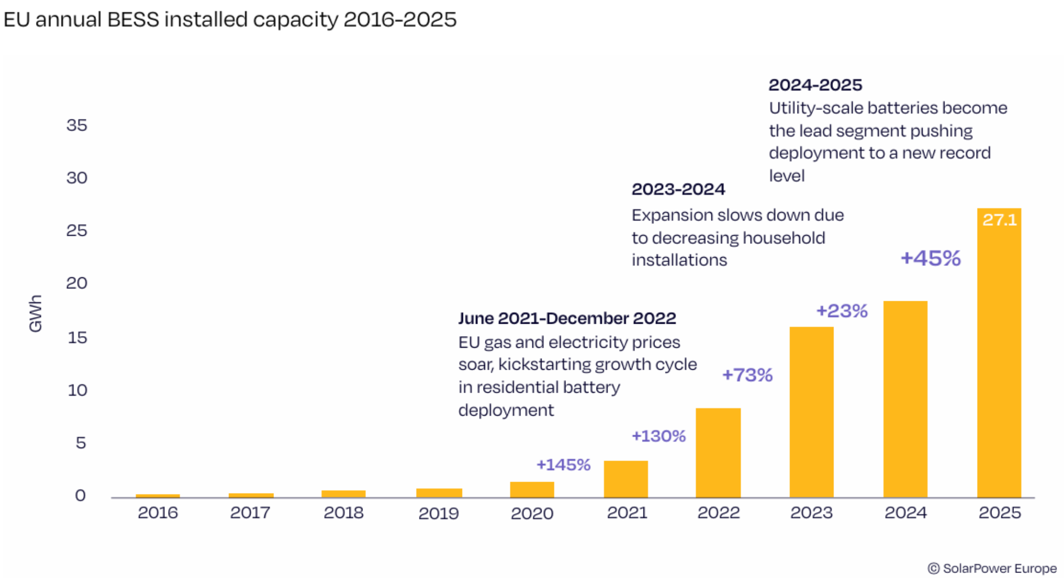
Commercially available aqueous NIBs

Natron Energy uses PBAs for both cathode and anode.

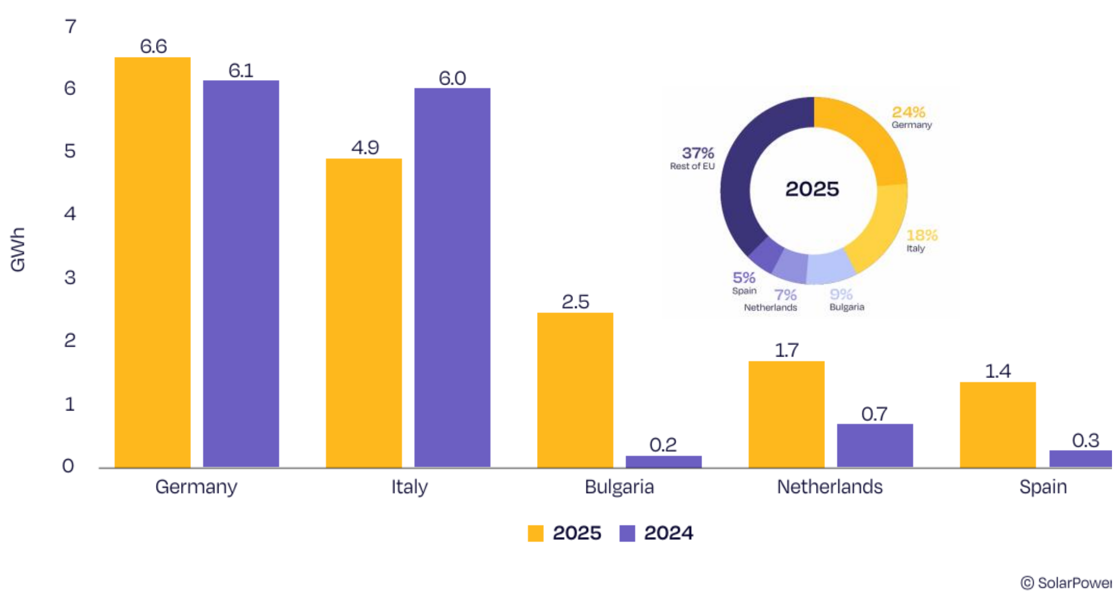
- Power > 750 kW and > 500 kW at run times of 1 and 2 min respectively,
- 50000 cycles. Energy 27 kWh
- Recharge time <10 minutes and safety (Nonflammable)

T. Rojo et al., *Adv. Energy Mater.* 2020, 2002055.

Battery storage deployment in the EU



- In 2025, the EU installed 27.1 GWh of new battery energy storage systems (BESS).
- Utility-scale batteries became the main engine for growth, delivering 55% of all new capacity.



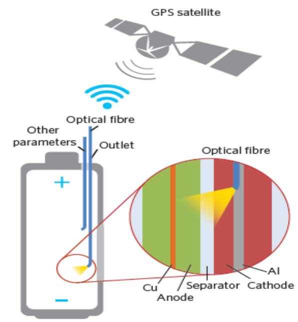
The cumulative installed battery capacity in the EU shows that the 5 largest battery markets capture nearly 70% of EU total capacity.

The vision and mission for BATTERY 2030+

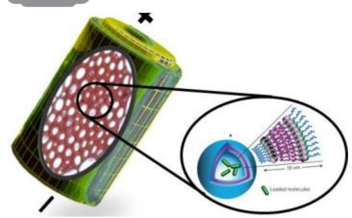
- **Europe needs** strategic investment now **to lead the discovery and manufacturing of ultrahigh-performance batteries.**
- Building upon its scientific excellence, Europe has the opportunity **to create a competitive industry for long-term prosperity and security.**
- Radically new approaches are needed **to accelerate the discovery of ultrahigh-performance materials and interfaces for the batteries of the future.**

"Smart batteries" and intelligent functionalities are key to next-generation technologies.

- ➢ Smart Batteries and sensing in a nutshell



- ➢ Battery self-healing (BSH) in a nutshell



Manufacturability, recyclability and sustainability.

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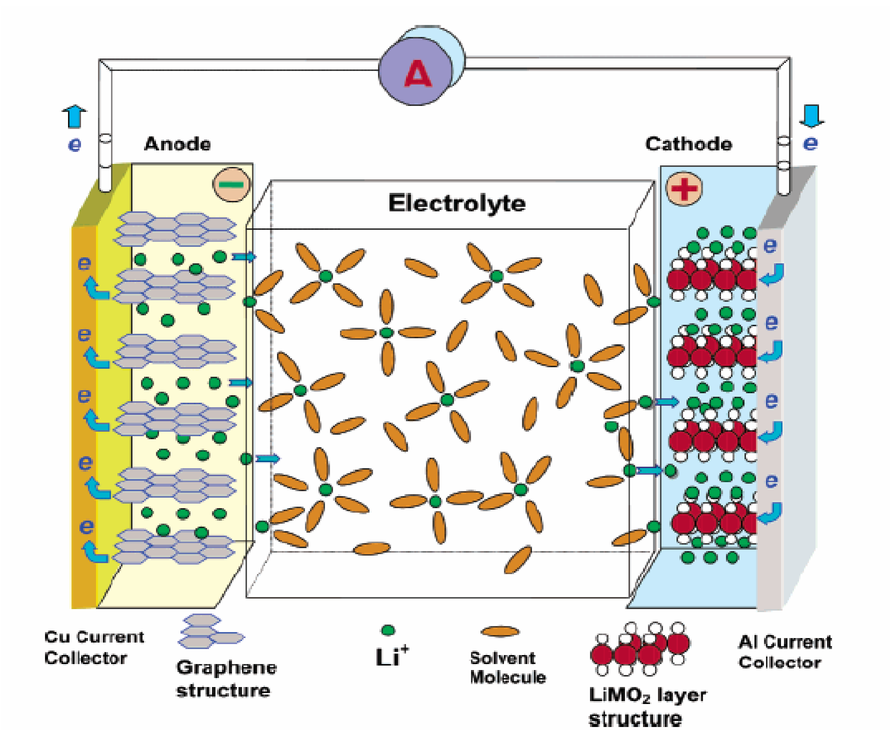
Electrochemical Energy Storage

Advanced Batteries

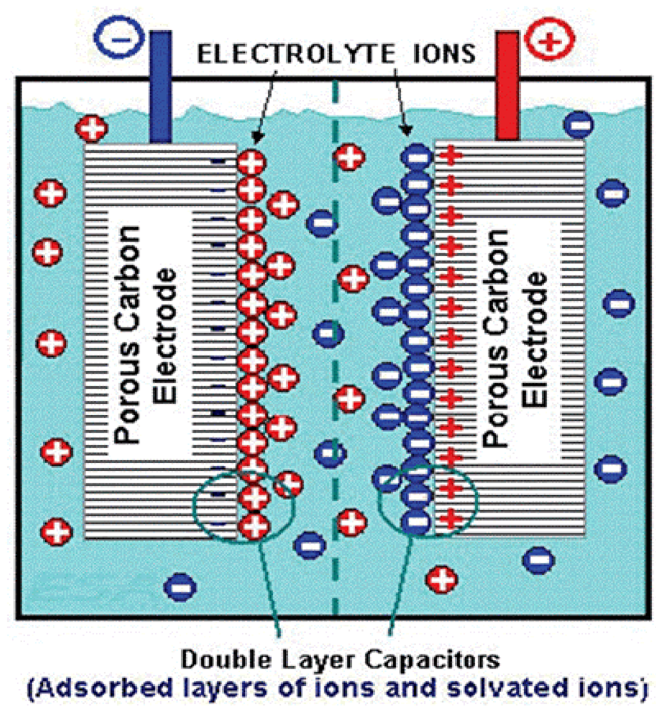
Electric energy is stored by the conversion of chemical energy through redox reactions between the anode and cathode.



US Department of Energy, 2007

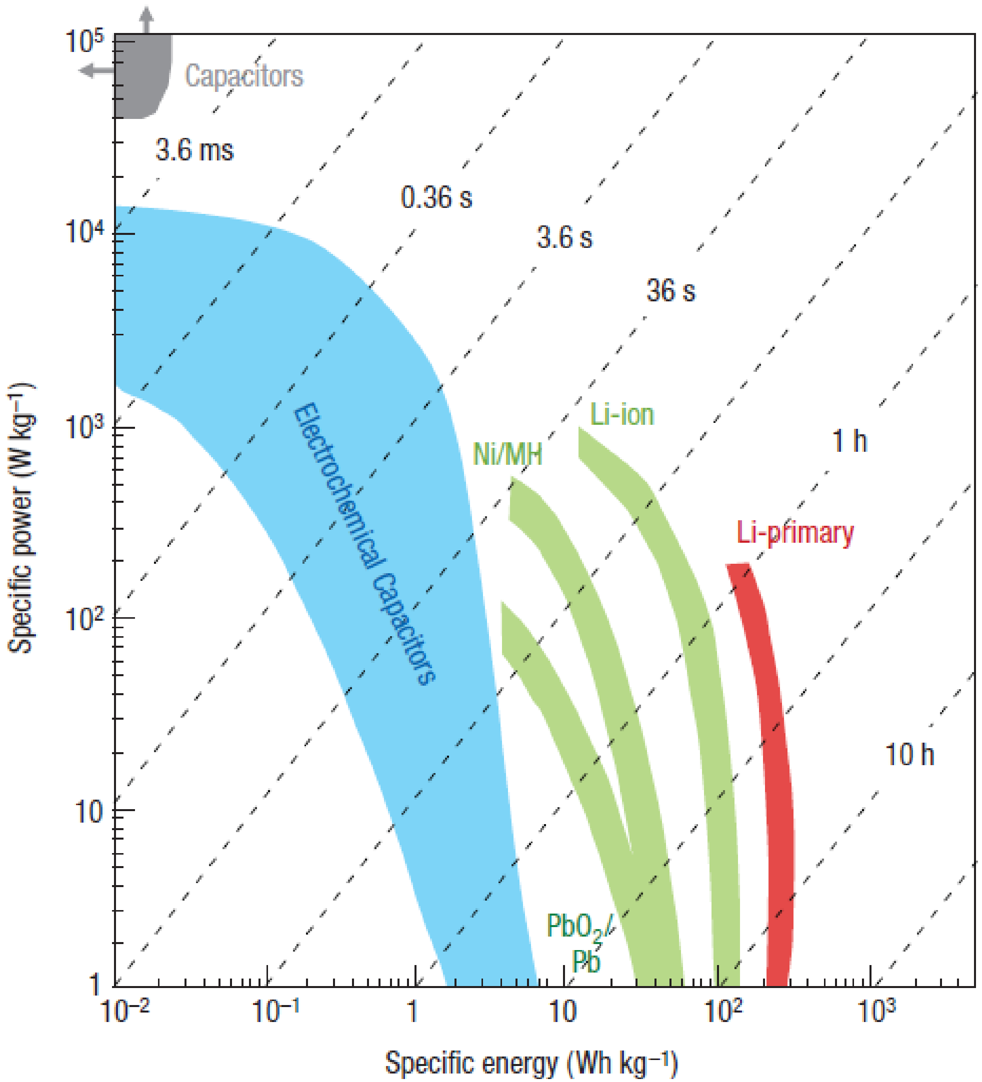
Supercapacitors

Electric energy is stored physically in the electrochemical double layer at the electrolyte-electrode interface.



http://www.ic.gc.ca/eic/site/wei-iee.nsf/eng/00177.html

Electrochemical Energy Storage



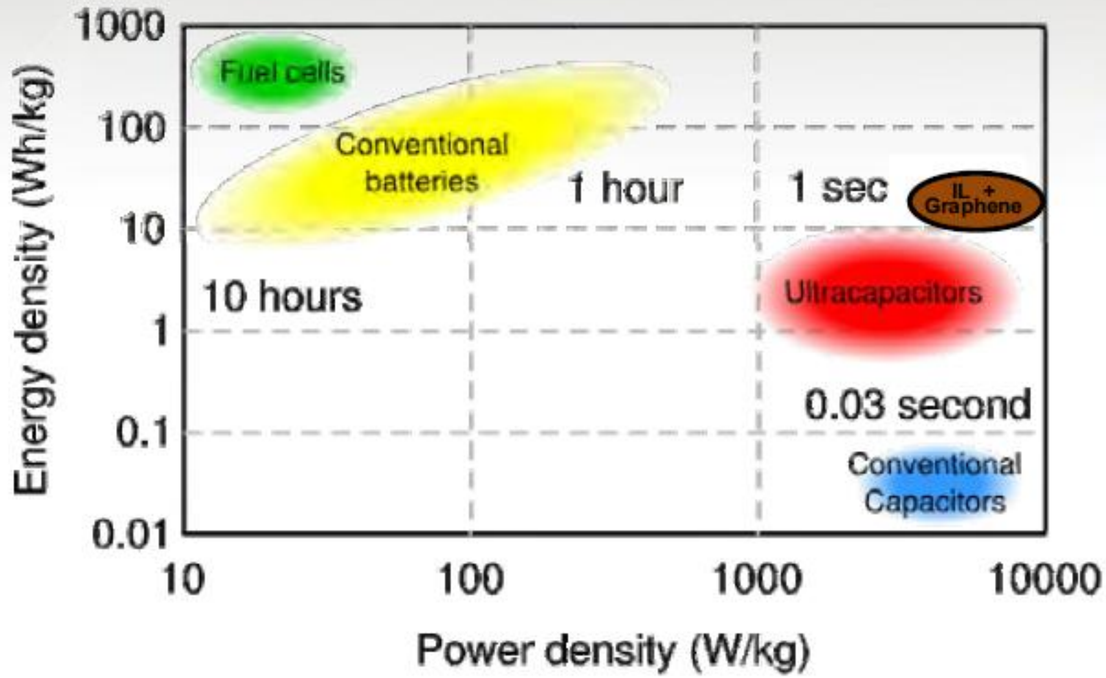
Advanced Batteries

- Higher energy density
- Lower power density
- Short cycle life
- Low self discharge

Supercapacitors

- Higher power density
- Lower energy density
- Long cycle life
- High self discharge

Battery vs. Ultracapacitors - *Costly, Bulky*



- Batteries store enough energy but they are slow, less efficient, and have limited cycle life
- Ultracapacitors are fast, efficient and have high cycle life but they are costly and bulky

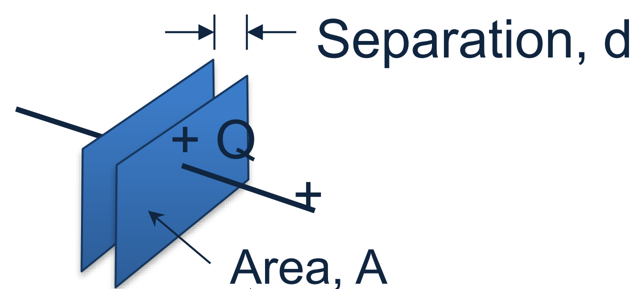
What´s a capacitor?

A Capacitor is a device that stores electric charge and electrical potential energy in an electric field. This ability is measured by the ***capacitance C***

$$C = \frac{Q}{V}$$

where C = Capacitance
Q = Stored charge
V = Electric potential

i.e. Capacitance is a measure of the ability of a device to store charge per unit of voltage applied across the device.



- **$C = \varepsilon\varepsilon_o A/d$**

  ε is electrolyte dielectric constant. ε_o is dielectric constant of the vacuum

- **Charge capacitor to voltage V**. Then charge Q is on plate

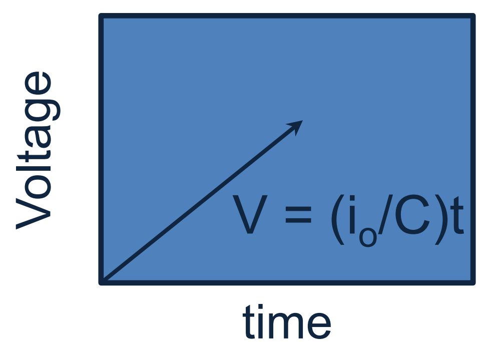
  $Q = C V$

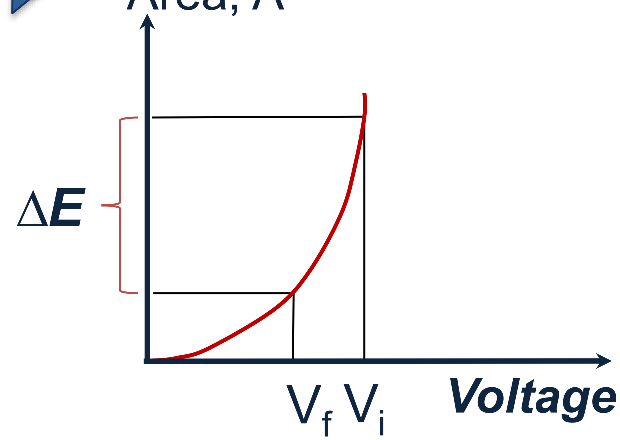
- **Charge capacitor at current i_o for time t**

  $Q = i_o t = C V \rightarrow V = (i_o/C)t$

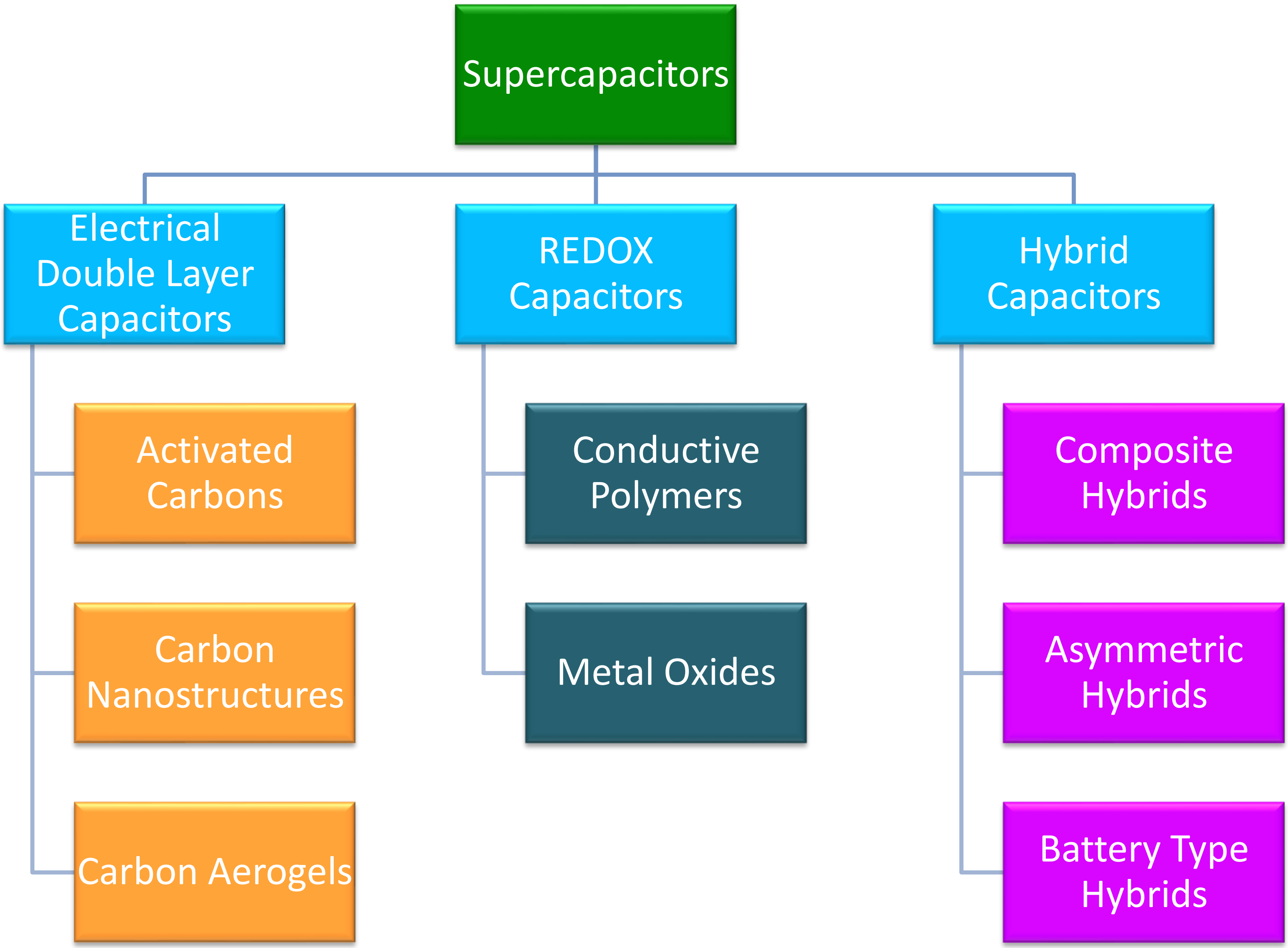
- **Energy in voltage window V_i to V_f**

  $\Delta E = ½ \, C \, (V_i^2 - V_f^2)$

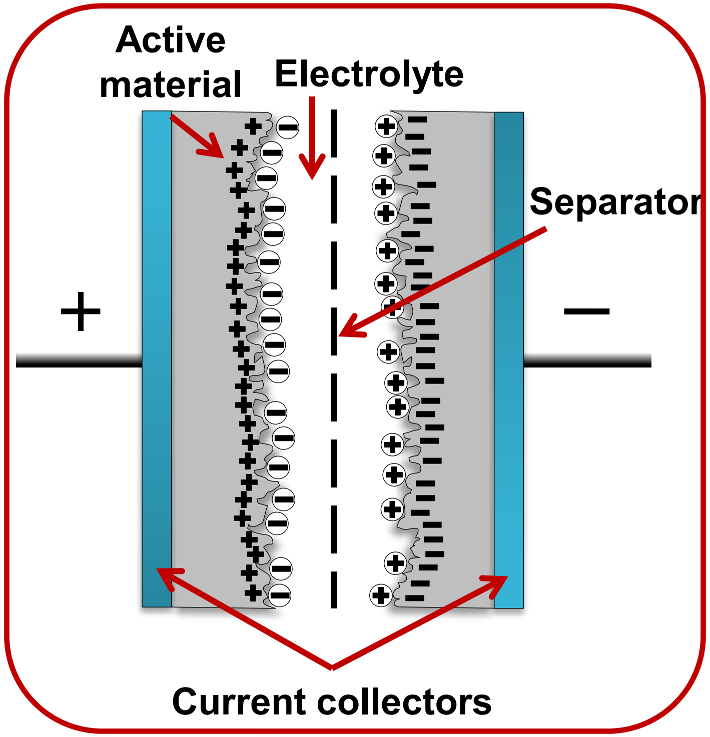


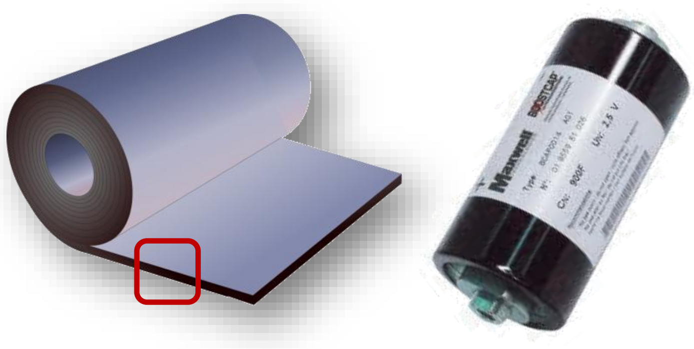


Classification of Supercapacitors



Electrochemical Double Layer Capacitors





Maxwell Technologies BoostCap

Carbon-based active materials with high surface area (1500 – 2000 m^2/g).

Aqueous electrolyte	Organic electrolyte
150 - 300 F/g	100 – 150 F/g
~ 1 V	~ 2.5 V

The stored energy is proportional to the capacitance and the squared voltage:

$$E = \frac{1}{2} C V^2$$

E ↗ ➔ **Capacitance ↗** and/or **Cell voltage ↗**

Graphene based Electrodes

$$E = \frac{1}{2} C V^2$$

	Porous activated carbon (AC)	Graphene derived from graphite oxide (GO)
Specific Surface Area	1000-2000 m^2/g	2400m^2/g (Theoretical : 2630m^2/g)
Gravimetric Capacitance	100-150 F/g	200 F/g
Energy Density	4-5 Wh/kg	70Wh/kg

2g of Graphene has surface area larger than a football field

EV Market with Supercapacitors

The CAF company uses systems based on a hybrid combination of **supercapacitors** and **lithium-ion batteries** in its **trams** that allow **circulation without catenary** in various cities such as Seville and Zaragoza

http://www.trainelec.com/enaccion.php

REDOX SUPERCAPACITORS
(Pseudo-capacitors)

▪ Undergo highly reversible redox (faradaic) reactions but behave like capacitors.

▪ Materials that exhibit pseudocapacitive storage range from conducting polymers to a variety of transition metal oxides.

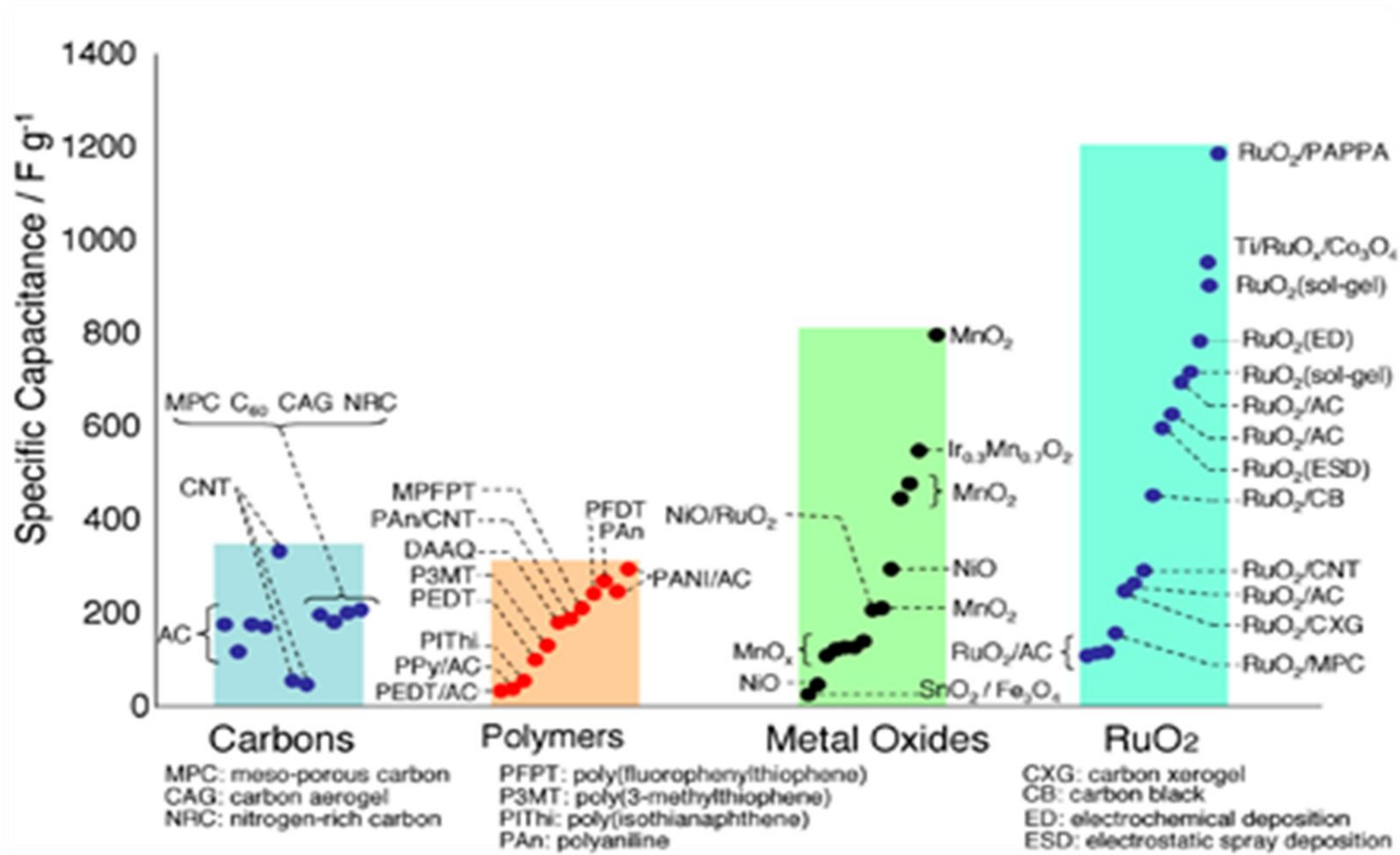
▪ Specific capacitance values as high as ~1000 F/g in aqueous electrolytes (more than 3 times higher than AC).

PseuodCap from Nesscap

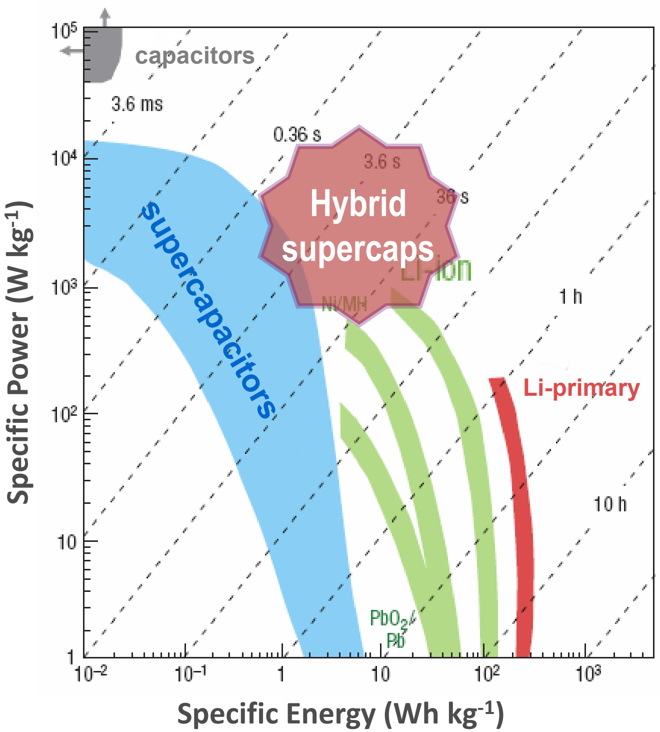
☹ Often suffer, like batteries, from a lack of stability during cycling.

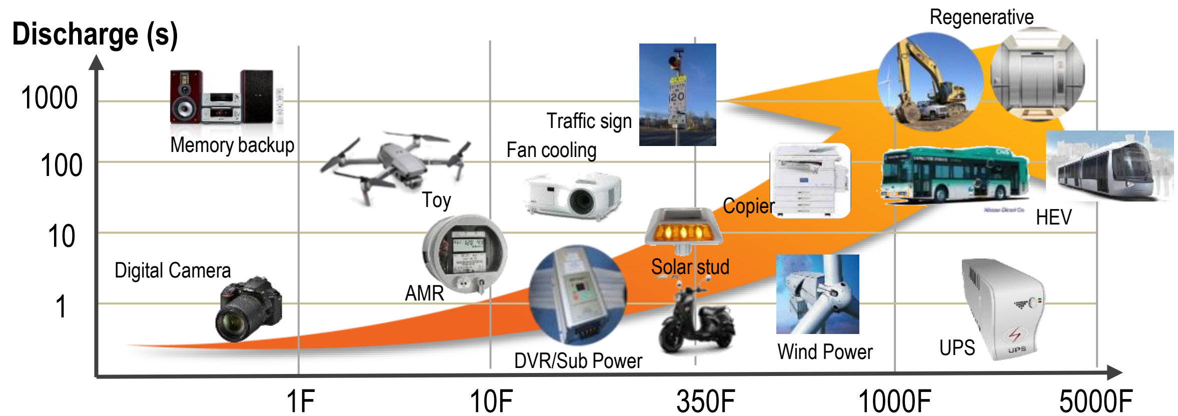
☹ Efforts to develop more practical pseudo-capacitive materials are now quite active.

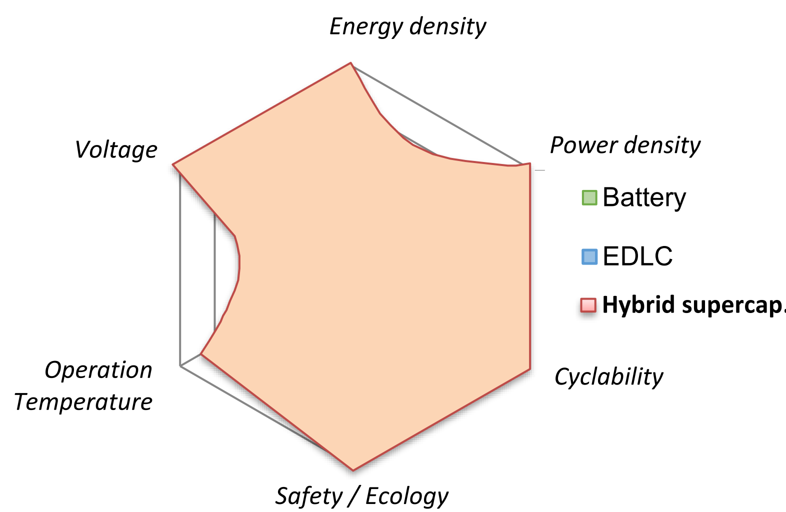
PSEUDO-CAPACITIVE MATERIALS



Hybrid supercapacitors







- ✓ High power: 10-20 kW kg^{-1}
- ✓ Specific Energy : 5 Wh kg^{-1}
- ✓ Time constant: 1 – 5 s
- ✓ Symmetric charge/discharge profile
- ✓ Cycle life > 1M cycles
- ✓ Broad temperature working range (- 40˚C)

Hybrid supercapacitors: Metal-ion capacitors MIC (M=Li,Na)

Commercial Li-ion capacitors

YUNASKO

2.7 V
1.3 Ah

Ukraine

ULTIMO® Laminate cell
2.2 V to 3.8 V
1100 F and 2100 F

Japan

JM energy JM Energy Corporation

ULTIMO®Prismatic cell
2.2 V to 3.8 V
3300 F and 2300 F

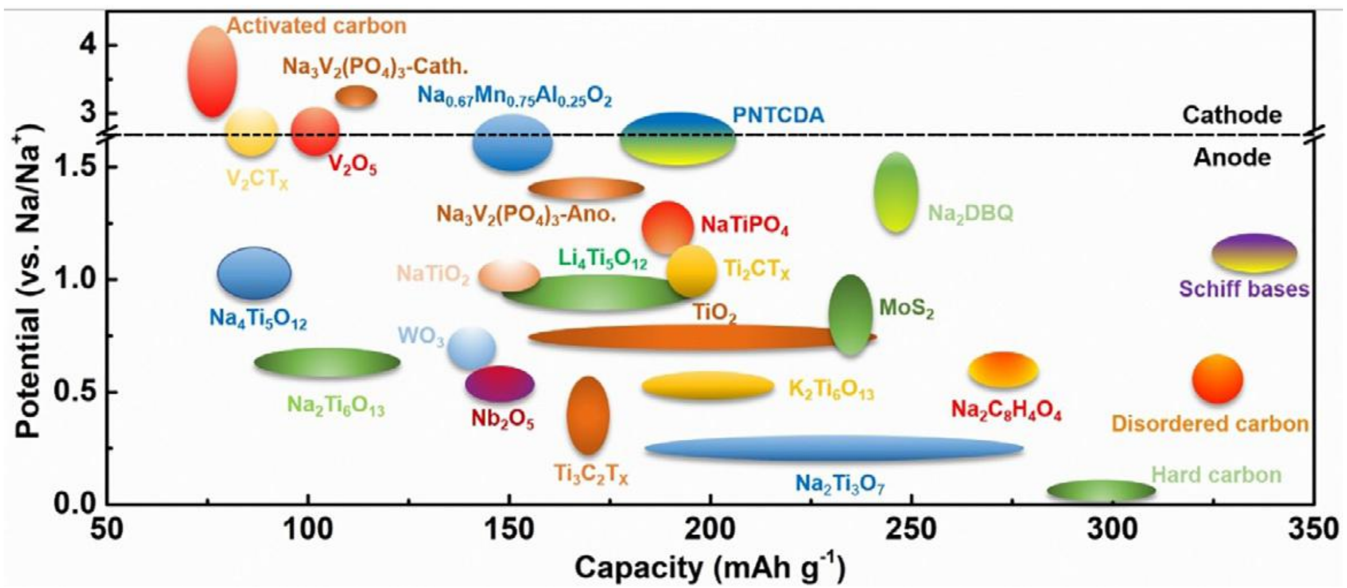
TAIYO YUDEN

2.2 V to 3.8 V
40 F to 270 F

Japan

Other manufacturers of LICs:

- Maxwell (USA)
- Murata (Japan), small LICs
- Anhui Aowei (China), large LICs



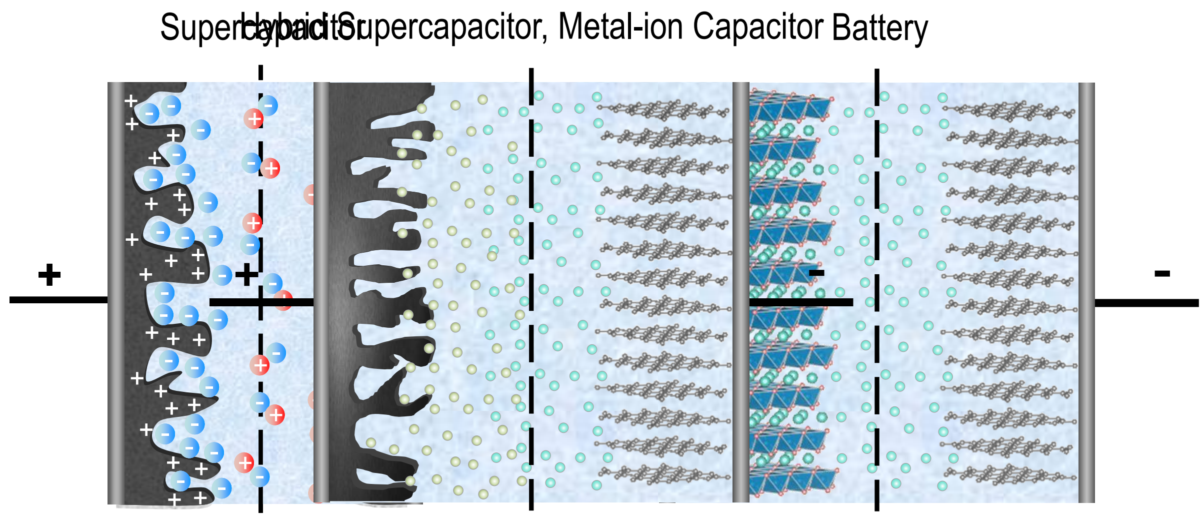
Still no commercial Na-ion capacitor

Area is ripe for exploitation – needs research dedication....

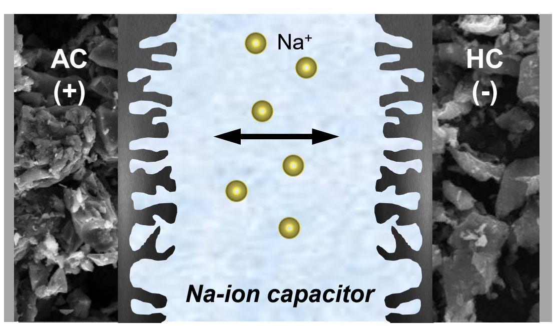
Z.Guo et al. *ChemSusChem* 2020, 13, 2522 – 2539

Na-ion hybrid capacitors

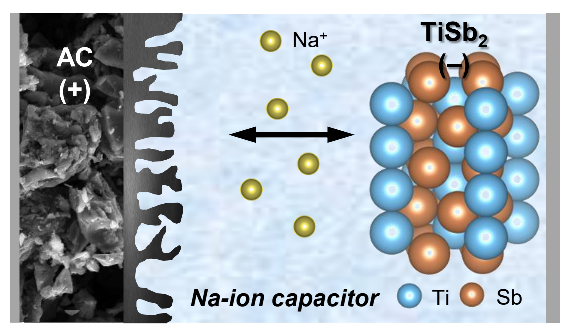
- **From energy to power density:**
  - Na-ion hybrid capacitors (NICs): high rate capability and power density.



Cell configurations

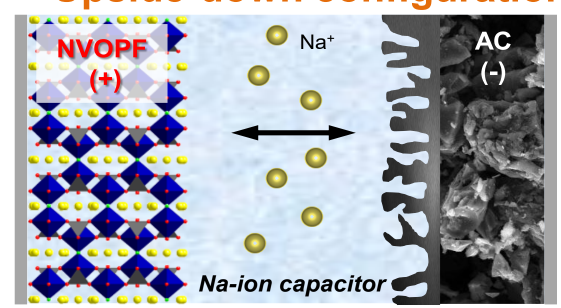


All carbon-based NIC



Alloy (-) & carbon-based (+) NIC

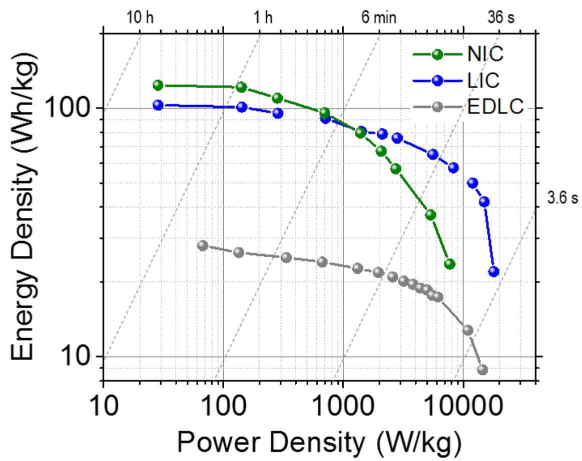
Upside-down configuration



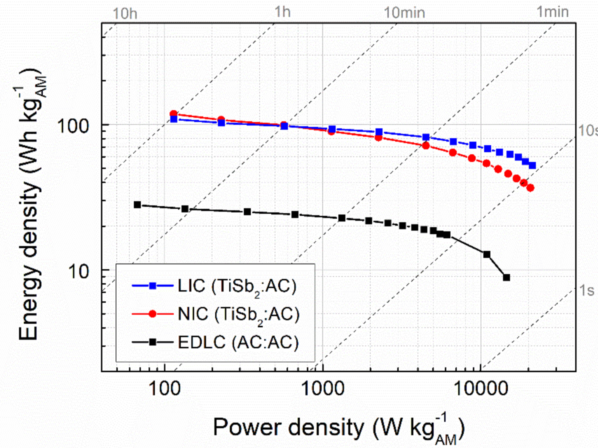
NVOPF (+) & carbon-based (-) NIC

HC/AC LIC vs NIC electrochemical performance

HC/AC LIC vs NIC

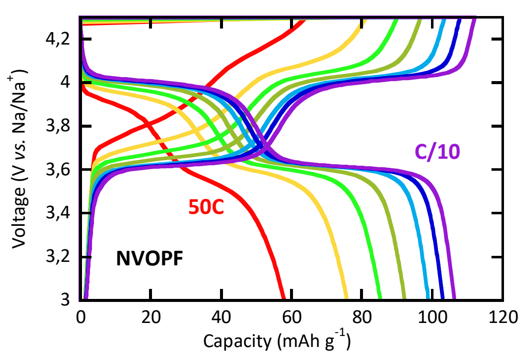


$TiSb_2$/AC LIC vs NIC

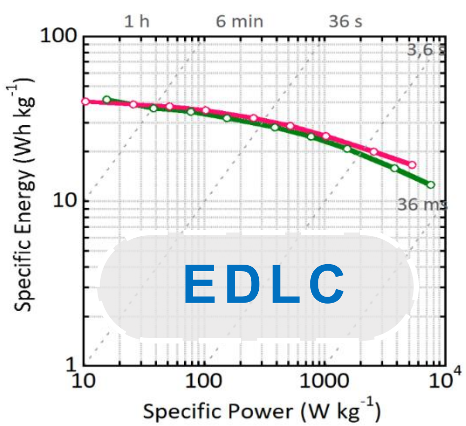


- The hybrid LIC and NIC devices overcome their EDLC counterpart in terms of energy density throughout the whole power density range.
- Both technologies equal the EDLC system in terms of power density (> 10 kW kg^{-1}) , showing the ability to be charged and discharged within a few seconds.

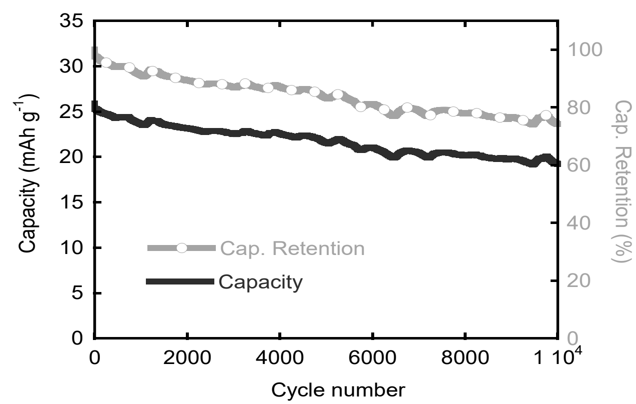
AC/NVOPF NIC



$Na_3V_2O_2(PO_4)_2F$, 60 mA h g^{-1} at 50C, can be used as positive electrode.



About twice de energy of an EDLC system.

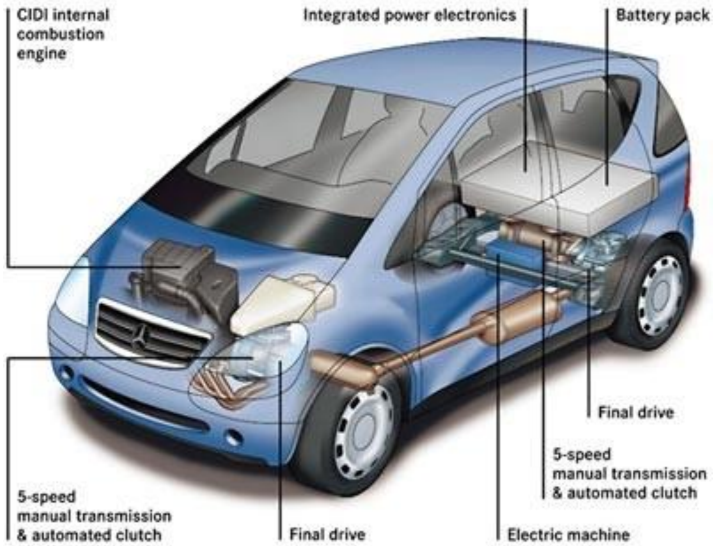


80% capacity retention at 10000 cycles

Supercapacitors *versus* batteries for vehicle applications

For HEV applications:

- Batteries alone and ultracapacitors alone can be an option.
- The decision might be based on cycle life and cost, in addition to relative power capability.



For PHEVs and EVs:

- The best option: ultracapacitors in combination with batteries designed for high energy density, long cycle life, and low cost.
- Combining the batteries and ultracapacitors can permit the use of high energy density batteries with insufficient power capability to be used alone.

A. Burke, M. Miller, *Journal of Power Sources* **196,** *514–522* (2011)

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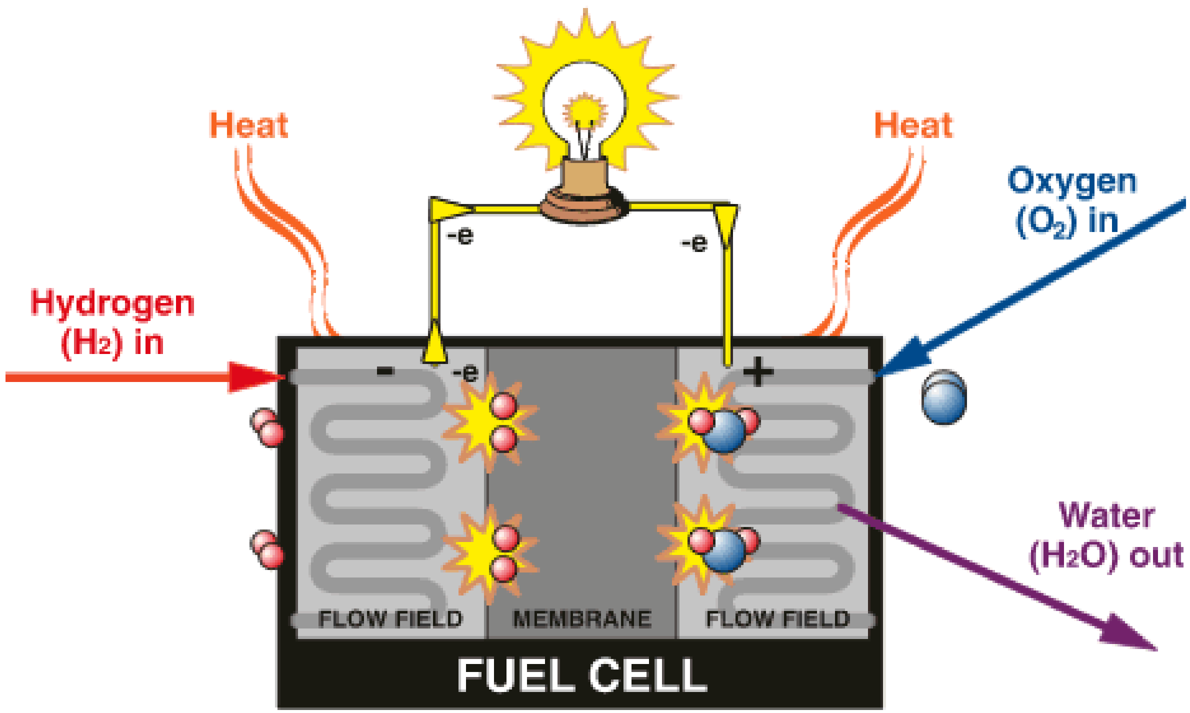
  - Electromobility
  - Stationary energy storage
- Materials for supercapacitors
  - Double layer capacitors
  - Pseudocapacitors
  - Hybrids
- Materials for Full Cells
  - Hydrogen as energetic vector
  - Electrolyzers
  - Mobility
- Summary and conclusions

FUEL CELLS

Direct energy conversion device, capable of transforming the chemical energy of a fuel into electrical energy.

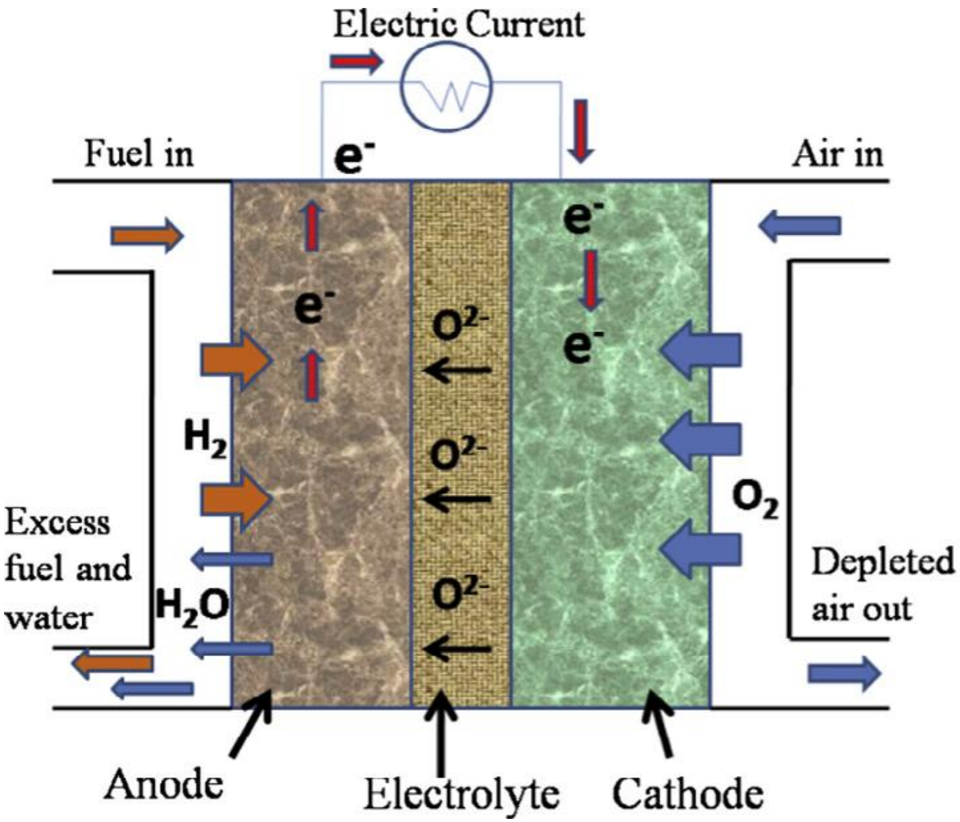


Fuel and oxidant are supplied continuously. In principle, the fuel cell produces power for as long as fuel is supplied.

Types of fuel cell based on electrolytes

Types of cells	alkaline	Methanolic	Molten carbonate	phosphoric	polymeric	Solid oxide
Electrolyte	Potassium hydroxide	Polymer membrane	Molten carbonate	Phosphoric acid	Replacemet membrane	ceramic
Operating temperature ºC	60–90	60–130	600-750	160 – 220	60-120	600-1200
Yield (%)	40–60	40	45–60	35–40	40–60	50–65
Production power	Up to 20 kW	Less than 10 kW	More than one kilowatt	More than 50 kW	up to 25 kW	More than 200 kW
Application	Submarine, Space	Portable applications	power plant	power plant	Vehicles, power plant	power plant

Solid oxide fuel cell (SOFC)



Oxide ion conductor electrolyte

This devise operates at high temperaturas (600-1200°C)

The important issue which controls **the whole process mainly depends on the material performance** during operational temperatures.

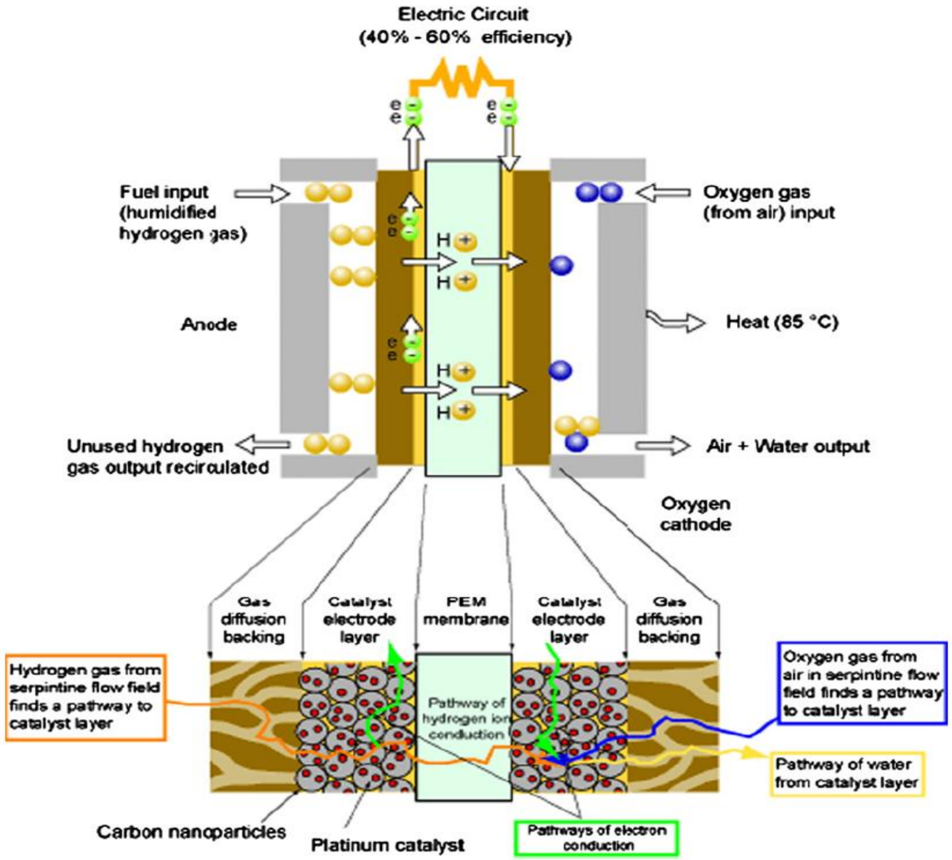
With the aim of decreasing temperature, material cost and improving stability, **new materials such as composites, nanostructured materials,..** should be developed.

Anode: Ni-O/YSZ (YSZ=$(ZrO_2)_{1-x}(Y_2O_3)_x$, CuO_2/CeO_2/YSZ, $La_{1-x}Sr_xMO_3$ (M=Mn,Co,Fe), CeO_2/GDC, TiO_2/YSZ ,

Cathode: $La_xM_{1-x}M'O_3$ (M=,Sr,Ba; M´=Mn,Co,Fe,); $Gd_xSr_{1-x}CoMO_3$ (M=Co,Mn,), $Pr_xM_{1-x}MO_3$ (´M=Ca, Ba, M´=Mn,Co) $LaNi_{1-x}Co_xO_3$, $Bi_2Sr_2CaCuO_8$ $Y_{1-x}Sr_yCo_yFe_{1-y}O_3$, $SrTi_{0.3}Fe_{0.63}Co_{0.07}O_{3-\delta}$, $Sr_{0.9}Ce_{0.1}Fe_{0.8}Ni_{0.2}O_{3-\delta}$ La_2MO_4 (M=Ni,Co,Mn,Cu),

Electrolyte: $(ZrO_2)_{1-x}(Y_2O_3)_x$, $(ZrO_2)_x(Sc_2O_3)_{1-x}$, $Ce_xM_{1-x}O_y$ (M= Gd, Sm,Y) ; $La_xSr_{1-x}Ga_yMg_{1-y}O_3$, $La_xSr_{1-x}Ga_yMg_{1-y-z}Co_zO_3$, $La_xSr_{1-x}Ga_yMg_{1-y-z}Fe_zO_3$, $La_{0.8}Sr_{0.2}Ga_{0.32}Mg_{0.08}Co_{0.2}Fe_{0.2}O_3$, $BaCe_xY_{1-x}O_3$.

Polymer Electrolyte Membrane Fuel Cells (PEMFC)



Phenomena in a PEMFC: two-dimensional sectional view

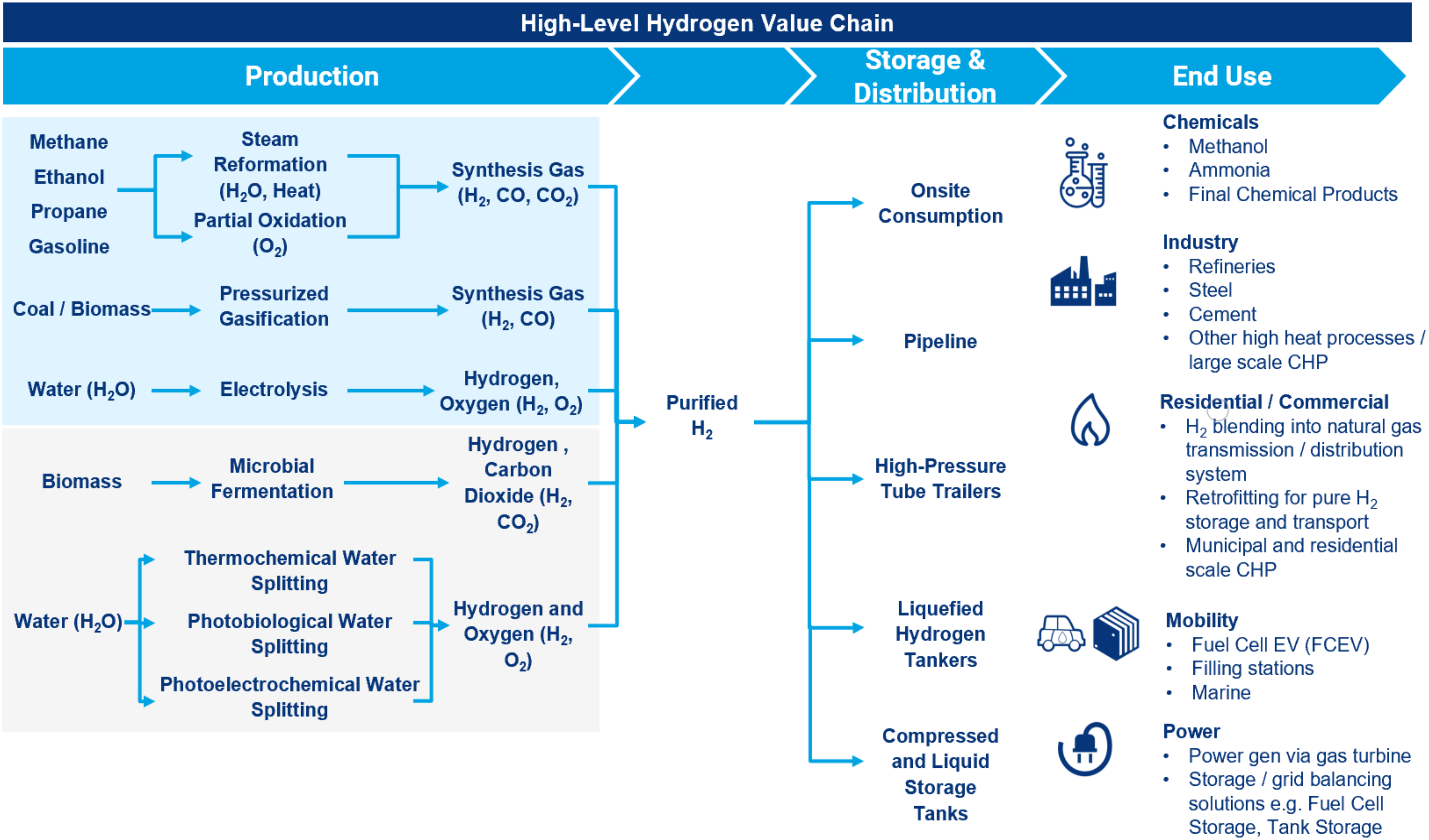
This devise operates at low temperaturas (< 60°C)

Reduction of cost by replacement of rare noble metal catalysts by **using molecular catalysts** e.g., metal–organic frameworks (MOFs), covalent organic frameworks (COFs) and molecular catalyst engineered polymers should be analyzed.

Catalyst: Pt , $[PMo_{(12-n)}V_nO_{40}]^{(3+n)-}$ (n = 0–3), Cu on Ru , Au (1 1 1), Pd/Co (90:10), $Mo_{4.2}Ru_{1.8}Se_8$

Electrolytes: acid-base polymer membranes, phosphoric acid-doped polybenzimidazole membranas, inorganic proton conductors, and organic-inorganic composite materials.

Why is hydrogen capturing a fashion?



It holds the promise to decarbonise so many “hard to abate” sectors

Source:Wood Mackensie 2021

Why do some people talk about colours of hydrogen?

In recent years, colours have been used to refer to different sources of hydrogen production:

- "**Black**", "**grey**" or "**brown**" refer to the production of hydrogen from coal, natural gas and lignite, respectively.

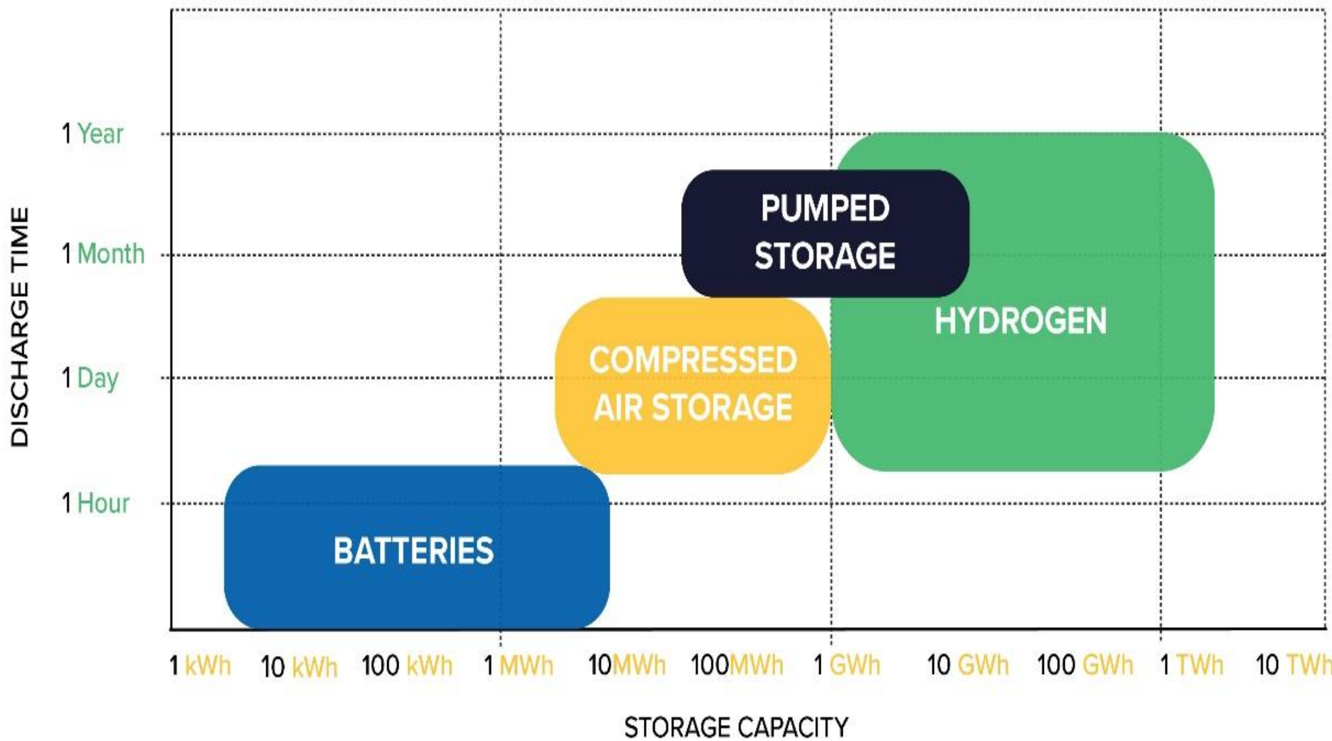
- "**Blue**" is commonly used for the production of hydrogen from fossil fuels with CO_2 emissions reduced by the use of carbon capture, utilization and storage (CCUS).

- **"Green"** is a term applied to production of hydrogen from renewable electricity.

- **"Red"** is recently applied to production of hydrogen from nuclear electricity.

- In general, there are no established colours for hydrogen from biomass or different varieties of grid electricity.

Could the Green Hydrogen Be Key to a Carbon-Free Economy?



- Hydrogen is abundant.
- Green hydrogen can be stored at scale.
- Green hydrogen can be produced from multiple renewable energy sources when operating as a reversed fuel cell. **Electrolyzers are needed.**

What is an electrolyzer and how does it work?

An electrolyzer is a system that uses electricity to break water into hydrogen and oxygen in a process called electrolysis.

There are different types of electrolyzers depending on their size and function:

- **Alkaline Electrolyzers**

Use a liquid electrolyte solution such as potassium hydroxide (KOH) or sodium hydroxide (NAOH), and water.

- **Proton Exchange Membrane (PEM) Electrolyzers**

Use a Proton Exchange Membrane and a solid polymer electrolyte.
PEM electrolysis consumes electricity and operate on the opposite principle to PEMFCs.

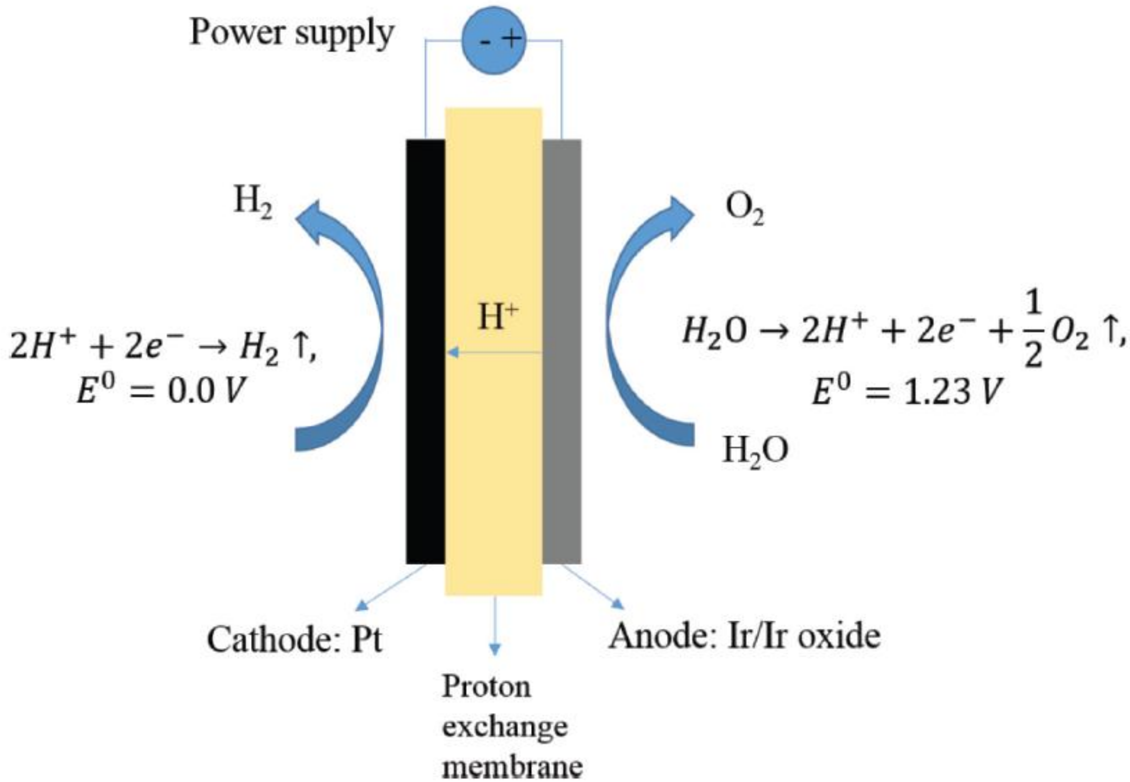
- **Solid Oxide Electrolyzers Cells (SOEC)**

Uses solid ceramic material as the electrolyte.
SOEC electrolysis consumes electricity and operate on the opposite principle to SOFC.

SOECs operate at a much higher temperature (above 500°C) than alkaline and PEM electrolyzers (up to 80°C) and have the potential to become much more efficient than PEM and alkaline. It is the most suitable technology for wider-scale adoption.

Proton Exchange Membrane (PEM) Water Electrolysis

When operated in reverse, a PEM functions as a polimeric membrane fuel cell (PEMFC)



- Avoid catalyst degradation in the electrochemical process.
- Utilize coatings on porous transport layers (PTL) to reduce contact resistance and passivation.
- The benefit of operating at lower overpotentials and temperatures (<80°C) can further help drive down the cost of the components.

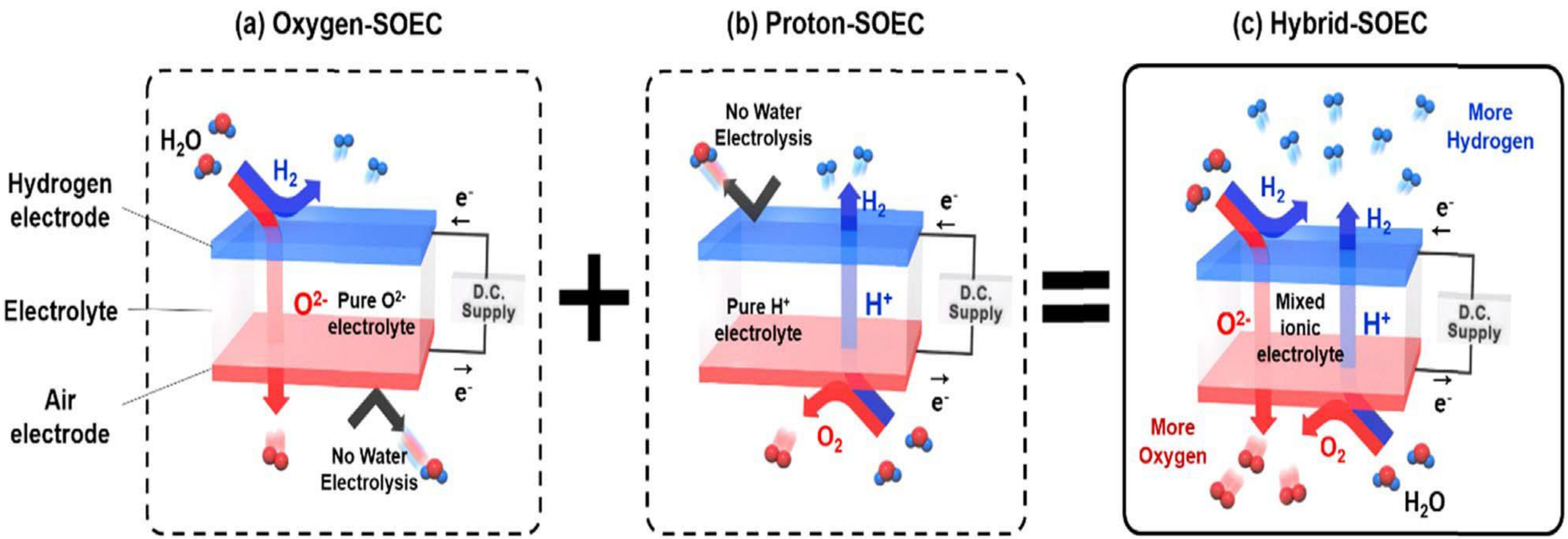
Electrocatalysts in PEM water Electrolysis

anode catalyst	cathode catalyst	anode loading (mg/cm^2)	cathode loading (mg/cm^2)	membrane	Temp (°C)
Ir-Black	40% Pt/GNF	2.0	0.8	Nafion-115	90
Ir-Black	40% Pt/XC-72	2.0	0.8	Nafion-115	90
Ir-Black	Pt40/Vulcan XC-72	2.4	0.7	Nafion-115	90
Ir-Black	Pd40/Vulcan XC-72	2.4	0.7	Nafion-115	90
Ir-Black	Pt-black	2.0	0.8	Nafion-117	90
IrO_2	Pt-black	2.0	2.5	Nafion-115	80
RuO_2	40% Pt/C	10	0.4	Nafion-115	–
RuO_2	30% Pt/C	3.0	0.5	Nafion-112	80
RuO_2	30% Pt/C	1.5	0.5	Nafion-1035	80
IrO_2	30% Pt/C	1.5	0.5	Nafion-1035	80
IrO_2	60% Pt/C	3.0	0.5	Nafion-115	80
IrO_2	30% Pt/C	2.5	0.5	Nafion-115	80
Ir-Black	Pt/CNT	2.4	–	Nafion-115	90
$Ru_{0.7}Ir_{0.3}O_2$	40% Pt/C	2.5	0.5	Nafion-117	80
IrO_2/SnO_2	40% Pt/C	1.5	0.5	Nafion-212	80
RuO_2/SnO_2	40% Pt/C	30.	0.6	Nafion-115	80
RuO_2	40% Pt/C	3.0	0.6	Nafion-115	80
RuO_2	30%Pd/N-CNT	3.0	0.7	Nafion-115	80
RuO_2	30%Pd/P-CNPs	3.0	0.7	Nafion-115	80
RuO_2	30%Pd/PG	3.0	0.7	Nafion-115	80
RuO_2	30%Pd/PN-CNPs	3.0	0.7	Nafion-115	80
$Ru_{0.8}Pd_{0.2}O_2$	30% Pt/CB	3.0	0.7	Nafion-115	80
$Ir_{0.6}Ru_{0.4}O_2$	20% Pt/C	2.04	2.04	Nafion-115	80
RuO_2	46% Pt/C	1.0	0.2	Nafion-117	80
$Ru_{0.9}Ir_{0.1}O_2$	46% Pt/C	1.0	0.2	Nafion-117	80
$Ru_{0.7}Ir_{0.3}O_2$	46% Pt/C	1.6	0.2	Nafion-117	80
$Ru_{0.3}Ir_{0.7}O_2$	46% Pt/C	1.4	0.2	Nafion-117	80
IrO_2	46% Pt/C	1.2	0.2	Nafion-117	80

Reduction of cost by replacement of rare noble metal catalysts by using molecular catalysts such as metal–organic frameworks (MOFs), covalent organic frameworks (COFs) and molecular catalyst engineered polymers, **is crucial**.

Solid oxide electrolysis cell (SOEC)

When operated in reverse, a SOEC functions as a solid oxide fuel cell (SOFC)



Hydrogen electrode:

$H_2O + 2e^- \rightarrow H_2(g, \text{water electrolysis}) + O^{2-}$

Air electrode:

$O^{2-} \rightarrow \frac{1}{2}O_2(g, \text{permeation}) + 2e^-$

Hydrogen electrode:

$2H^+ + 2e^- \rightarrow H_2(g, \text{permeation})$

Air electrode:

$H_2O \rightarrow 2H^+ + \frac{1}{2}O_2(g, \text{water electrolysis}) + 2e^-$

Hydrogen electrode:

$2H^+ + 2e^- \rightarrow H_2(g, \text{permeation})$

$H_2O + 2e^- \rightarrow H_2(g, \text{water electrolysis}) + O^{2-}$

Air electrode:

$H_2O \rightarrow 2H^+ + \frac{1}{2}O_2(g, \text{water electrolysis}) + 2e^-$

$O^{2-} \rightarrow \frac{1}{2}O_2(g, \text{permeation}) + 2e^-$

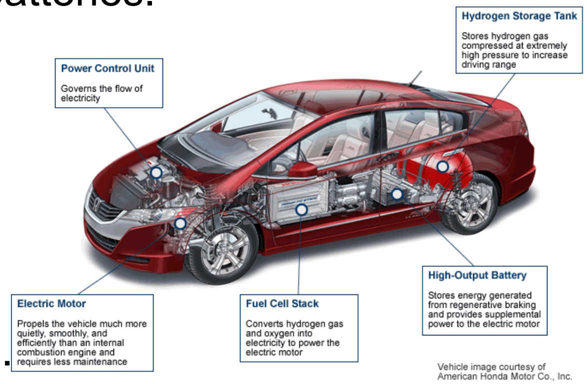
Schematic diagrams of the working principle. (a) Oxygen-SOEC, (b) proton-SOEC, and (c) Hybrid-SOEC operating system (**mixed ion conducting electrolyte $BaZr_{0.1}Ce_{0.7}Y_{0.1}Yb_{0.1}O_{3-\delta}$ is used**).

Hydrogen Vehicle Market with Fuel Cells

Polymeric membrane fuel cells (PEM-FC) generally used in hydrogen vehicles

Advantages:

- These devices have energy densities five times higher than lithium ion batteries.
- Recharging takes place in a couple of minutes.
- Driving ranges of 600-700 km and a route of more than 250.000 km



Disadvantages:

- Cost of materials, mainly catalysts.
- The integral hydrogen infrastructure (production, storage and transport).
- The lack of "*hydrogeneras*" that could involve an initial investment of more than three billion euros.

Hydrogen vehicles will be used primarily **for heavy vehicles** (trucks, trams, ships, planes).

In Europe the hydrogen infrastructure is very modest and along with its complexity and high cost the progress of incorporation of this type of vehicles in the coming years will be slow.

The Hydrogen Association of Spain considers that although there are currently **only six service stations**, which obtain their fuel through electrolysis, **in 2030 there will be more than 140000 vehicles circulating in this country.**

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    - Mobility
- Summary and conclusions

Summary and conclusions.

Batteries:

- Electrification and large energy storage are a great challenge.
- Batteries comprising most abundant and not toxic materials are required.
- Cost is the main barrier to expanding electrification. Energy (need 300 to 500 Wh/kg) can impact cost significantly.
- Smart Batteries with sensing and/or self-healing should be developed.

Supercapacitors:

- Supercapacitors are also good option: high power, low hysteresis, excellent cycle life, but the low voltage and low density are a big problem.
- Preparing activated carbons is also expensive.

Fuel Cells:

- The hydrogen will play a key role in a clean, secure and affordable energy future.
- New materials such as composites, nanostructured materials, molecular catalysts should be developed to improve performance and reduce cost in FCs.
- Technological advancement is still demanded in the field of electrocatalysis and material science to obtain a deeper understanding of catalytic reactions and design new catalysts.

Developing advanced materials is the key to clean energy and clean mobility technologies in the future and (due to industry 4.0) will soon account for 80% of the technology manufacturing cost.

Thank you for your kind attention!

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