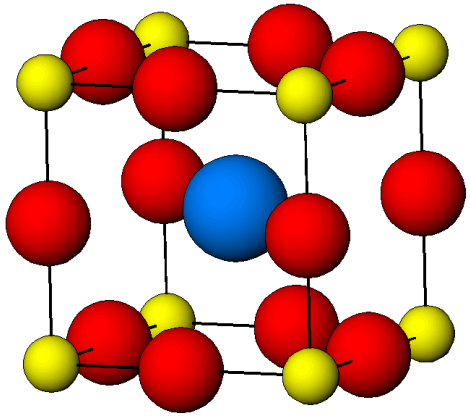
Saiful Islam
University of Oxford

Oxford Energy Day, March 2022

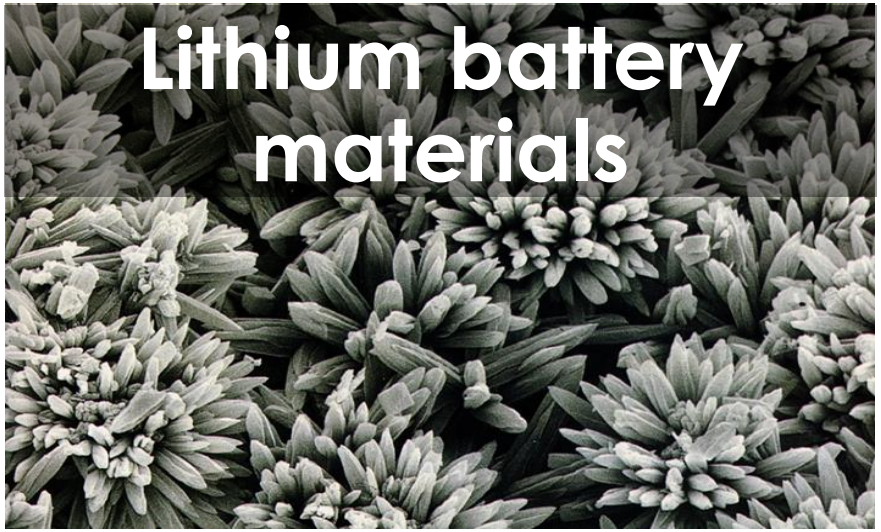
Making a Materials Difference to Batteries for Transport

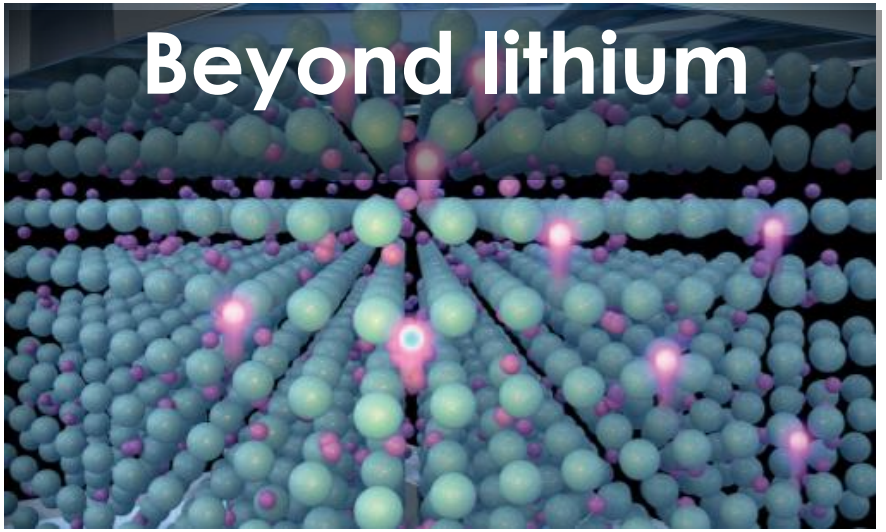


Menu


Energy storage


Batteries & EVs

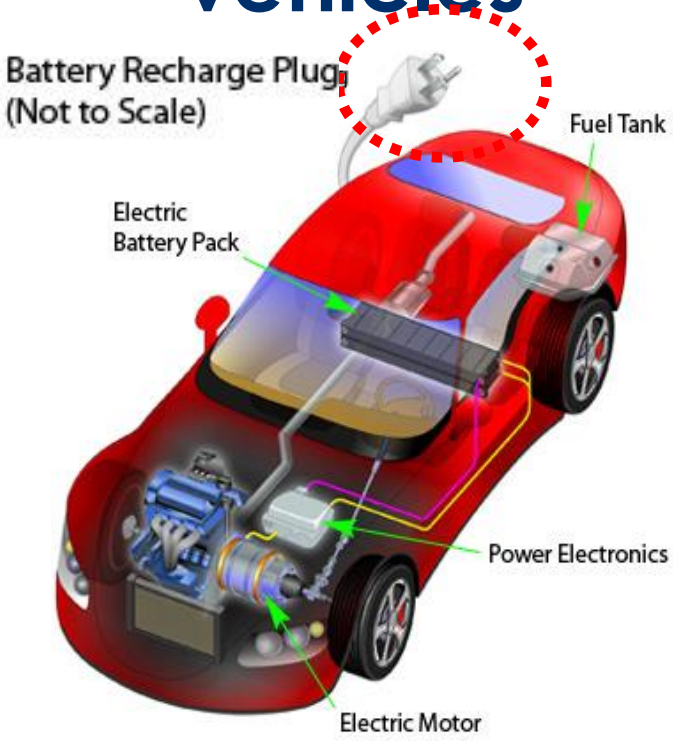

Lithium battery materials


Beyond lithium

Energy Storage & an Electrified Future

Portable electronics

Electric vehicles

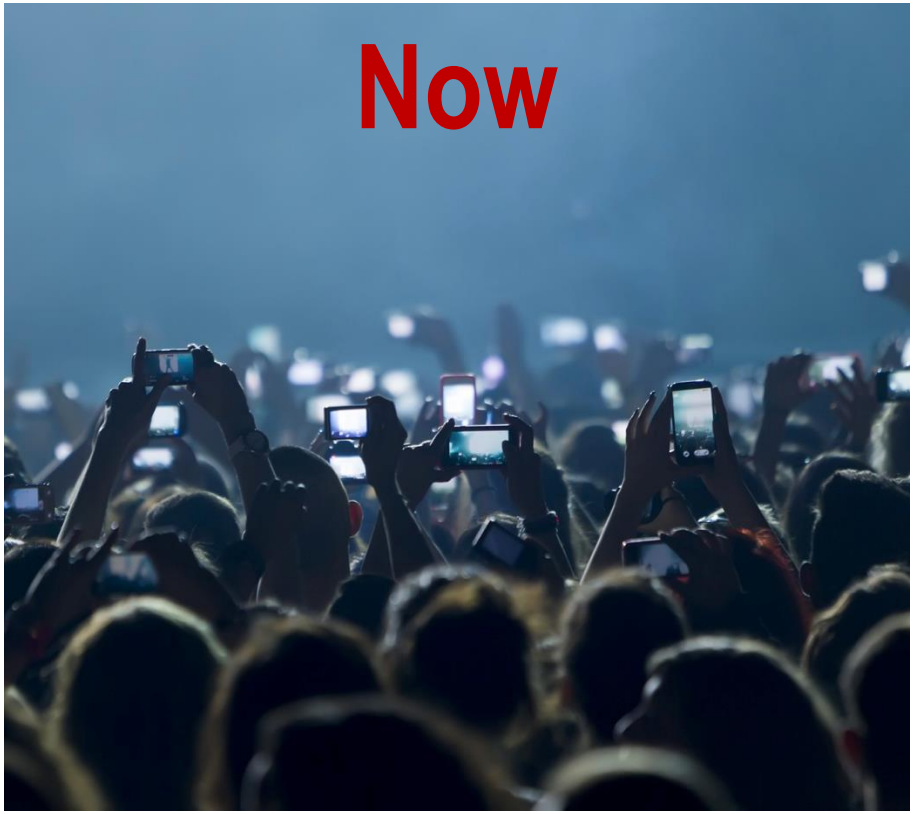


CO_2 emissions
Air quality

Grid storage

Intermittent renewables

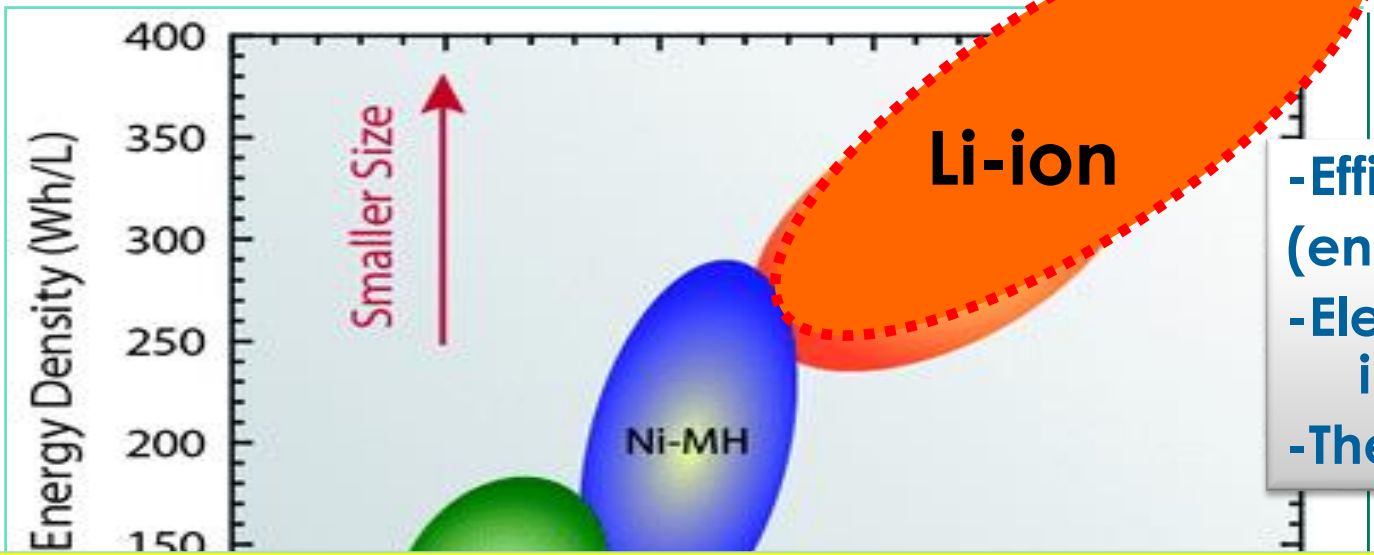
Portable Revolution



Powered by lithium-ion batteries

Batteries
& Electric Vehicles

Why power cars with lithium batteries?

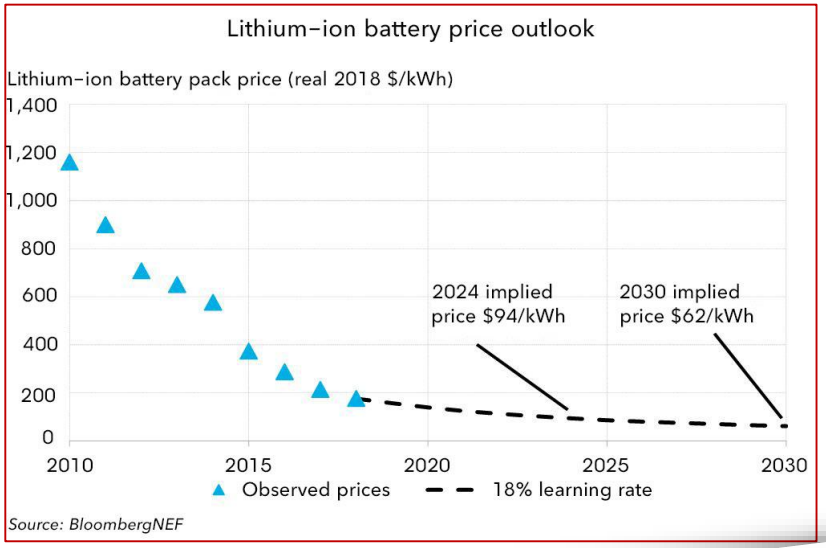


- Efficient (energy in/out 90%)
- Electricity infrastructure
- They work!

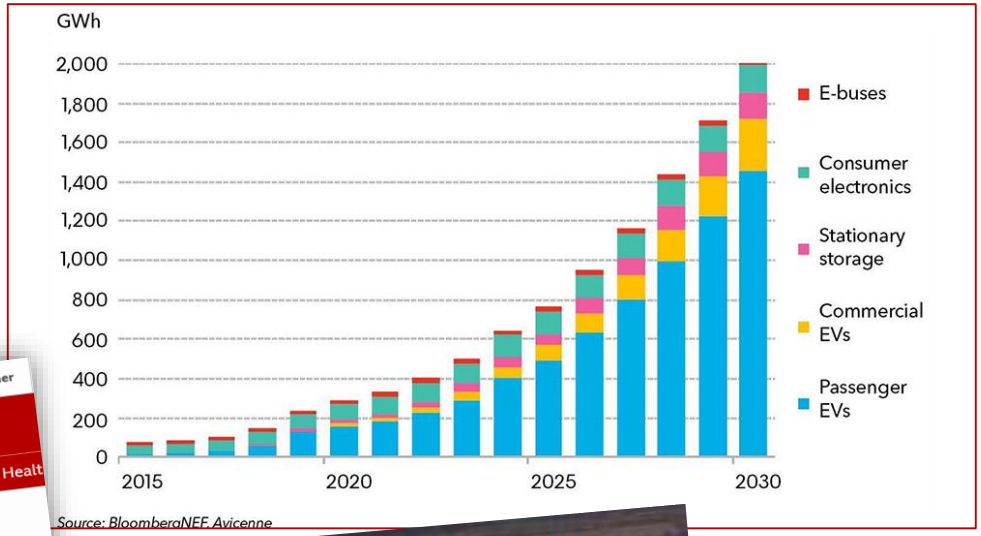
Step change advances?
New materials, innovation & underpinning science

Li-ion battery cost & market

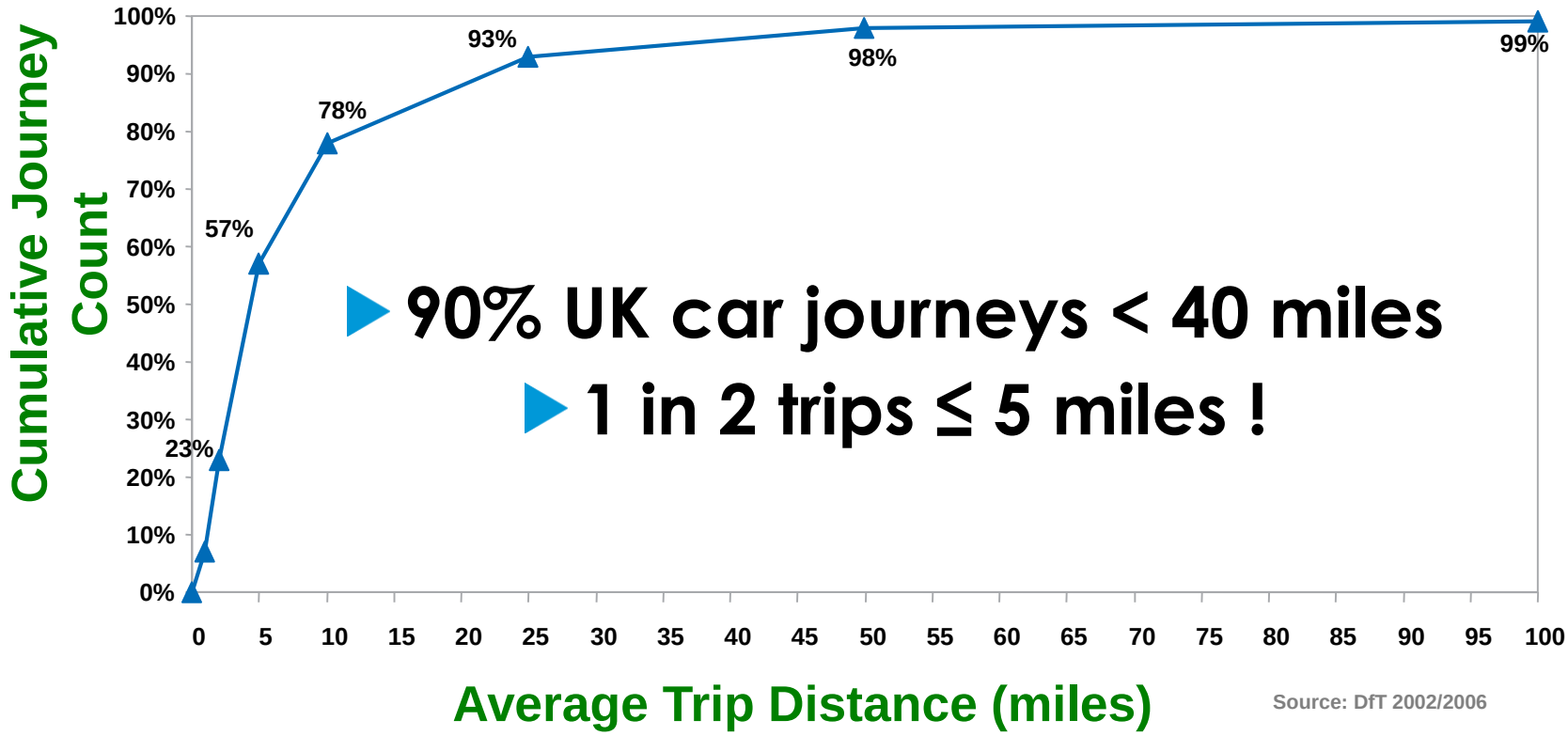
- Fall in battery pack price



- Battery market growth predicted - due to transition to EV



Range Anxiety? UK Car Journeys



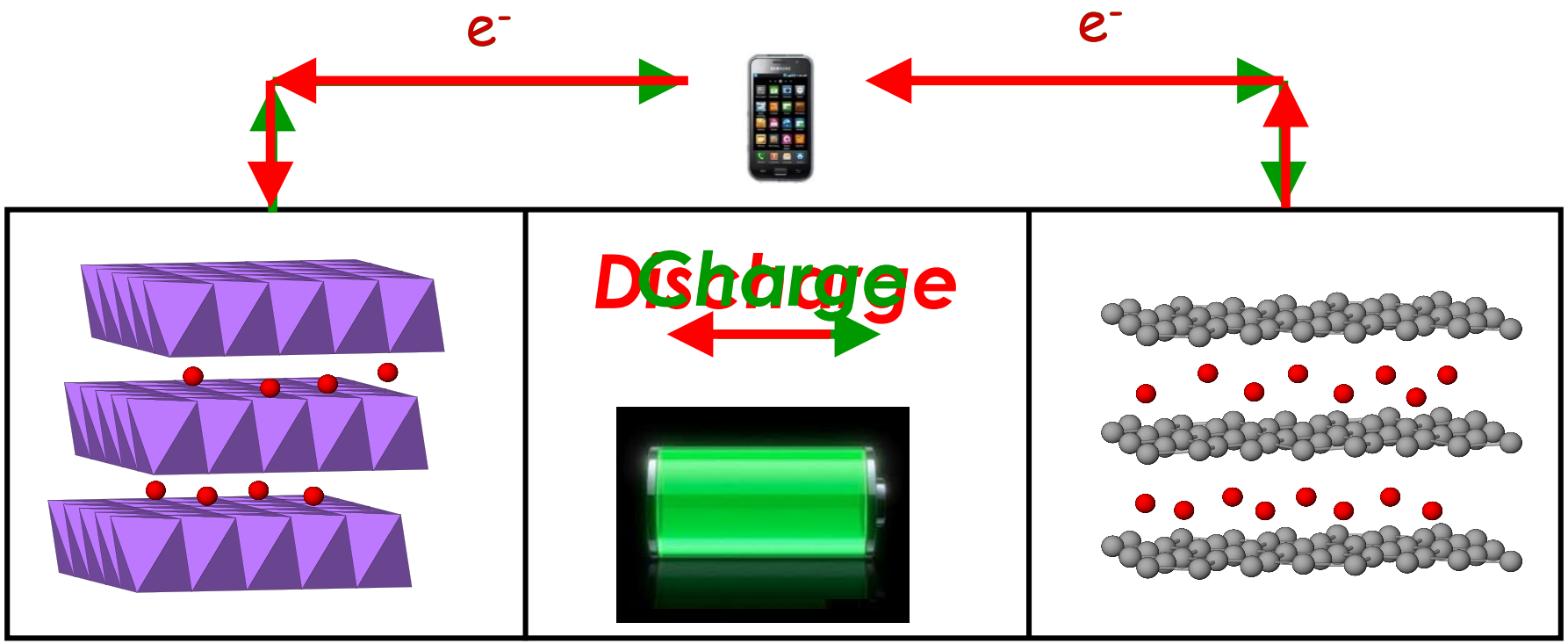
- 90% UK car journeys < 40 miles
- 1 in 2 trips ≤ 5 miles !

Source: DfT 2002/2006

D. Greenwood, WMG Warwick

Lithium Battery Materials

Inside a Lithium-Ion Battery



Nobel Prize 2019...long overdue!

John B. Goodenough
(Prof, Oxford, 1980s)

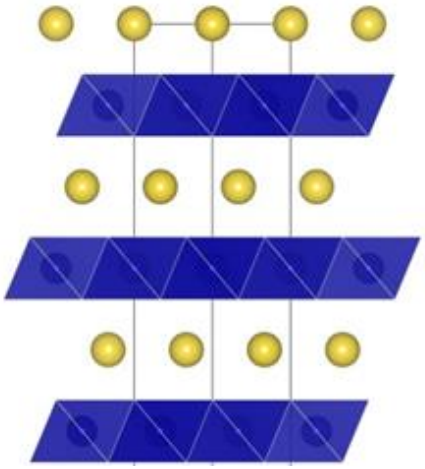
(BA/DPhil, Oxford,1960s)

Battery Materials: Cathodes

Materials Science is Critical

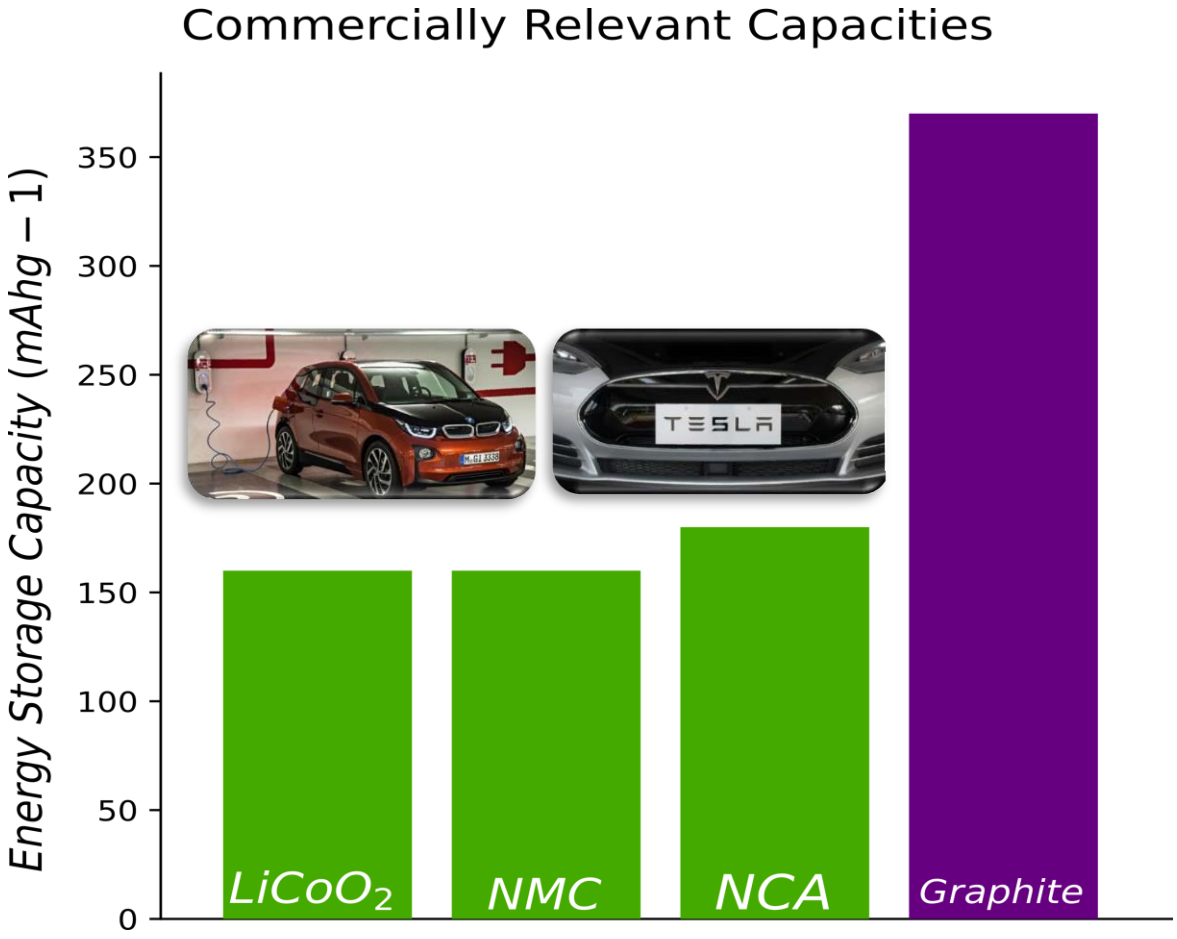
Cathode (oxide) vs Anode (graphite)

Lithium



Cobalt

NMC = Ni,Mn,Co



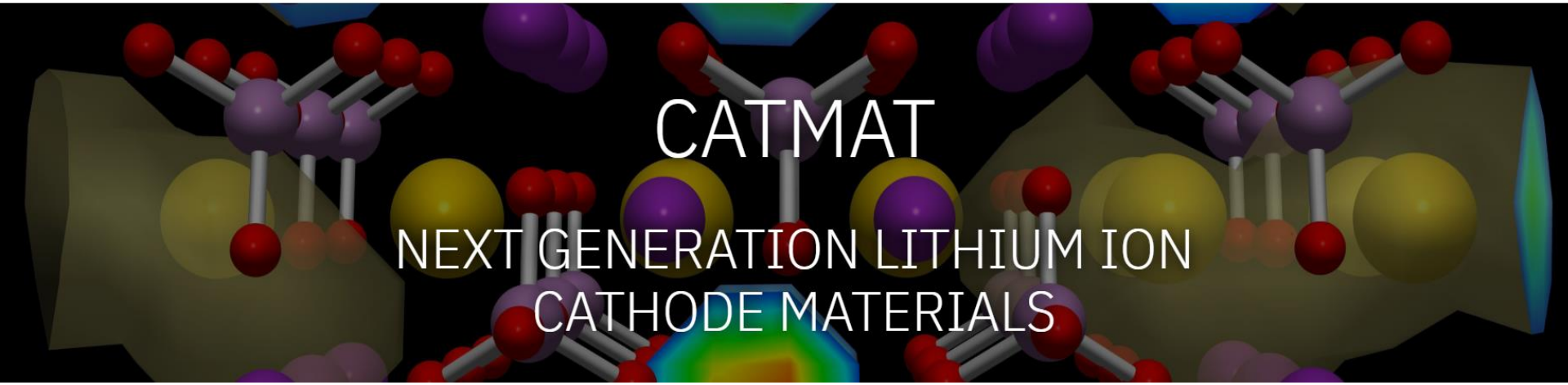
Next-Generation Cathodes

THE FARADAY INSTITUTION CATMAT

NEXT GENERATION LI-ION CATHODE MATERIALS

Home People Research Events News Contact

Catmatproject.com



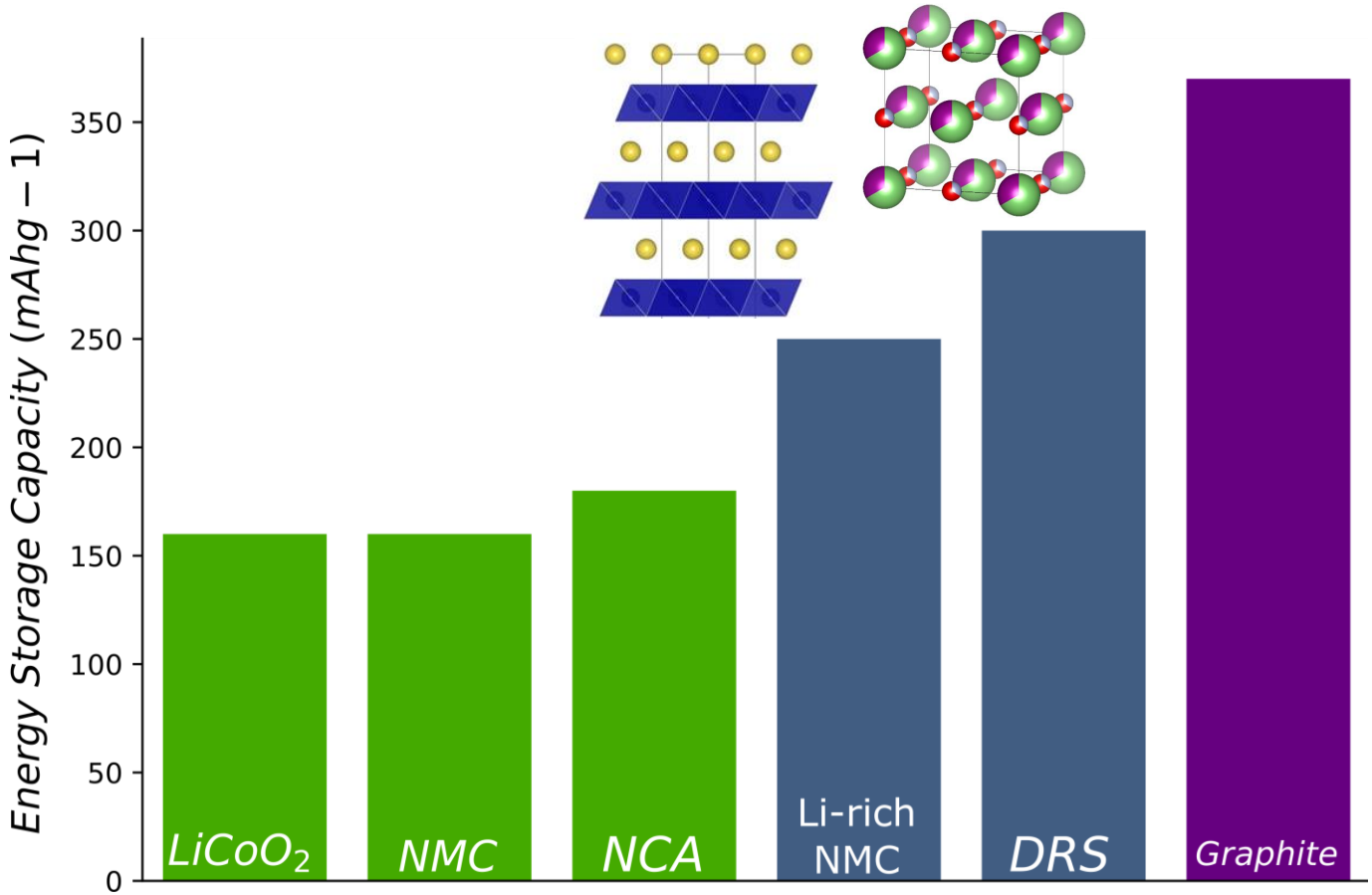
Lead (PI) **SI at Oxford Materials**

Team: **20 Postdocs, 12 PhDs**

Chemistry (Bath, Camb, Liver) + Engineering (Bham, UCL)

New Cathodes: O-Redox

- Conventional: store charge on transition metal
- Li-rich: Li/TM > 1

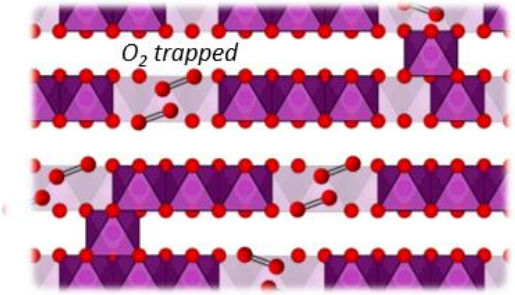


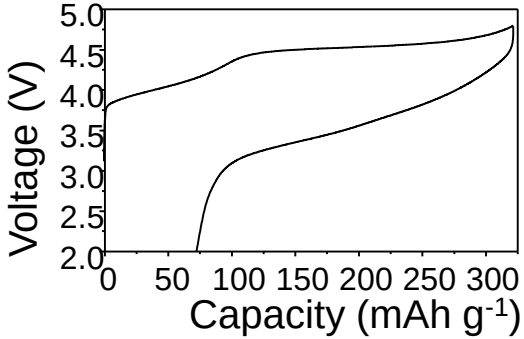
Layered & disordered rocksalt (DRS)

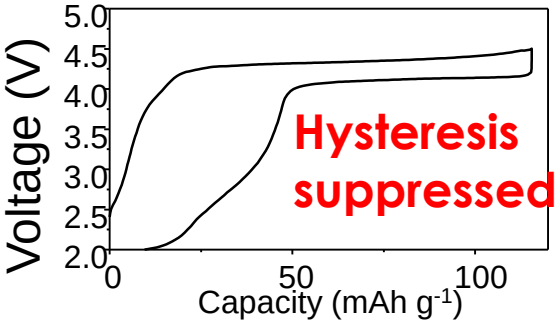
Away from Co Ni- or Mn-rich

O-Redox: Understanding & Design

- Challenge: 1st cycle voltage hysteresis in Li-rich NMC
- O-redox: O_2 trapped in bulk
- If TM ions ordered in ribbon arrangement - hysteresis suppressed
- HIGH VOLTAGE MAINTAINED







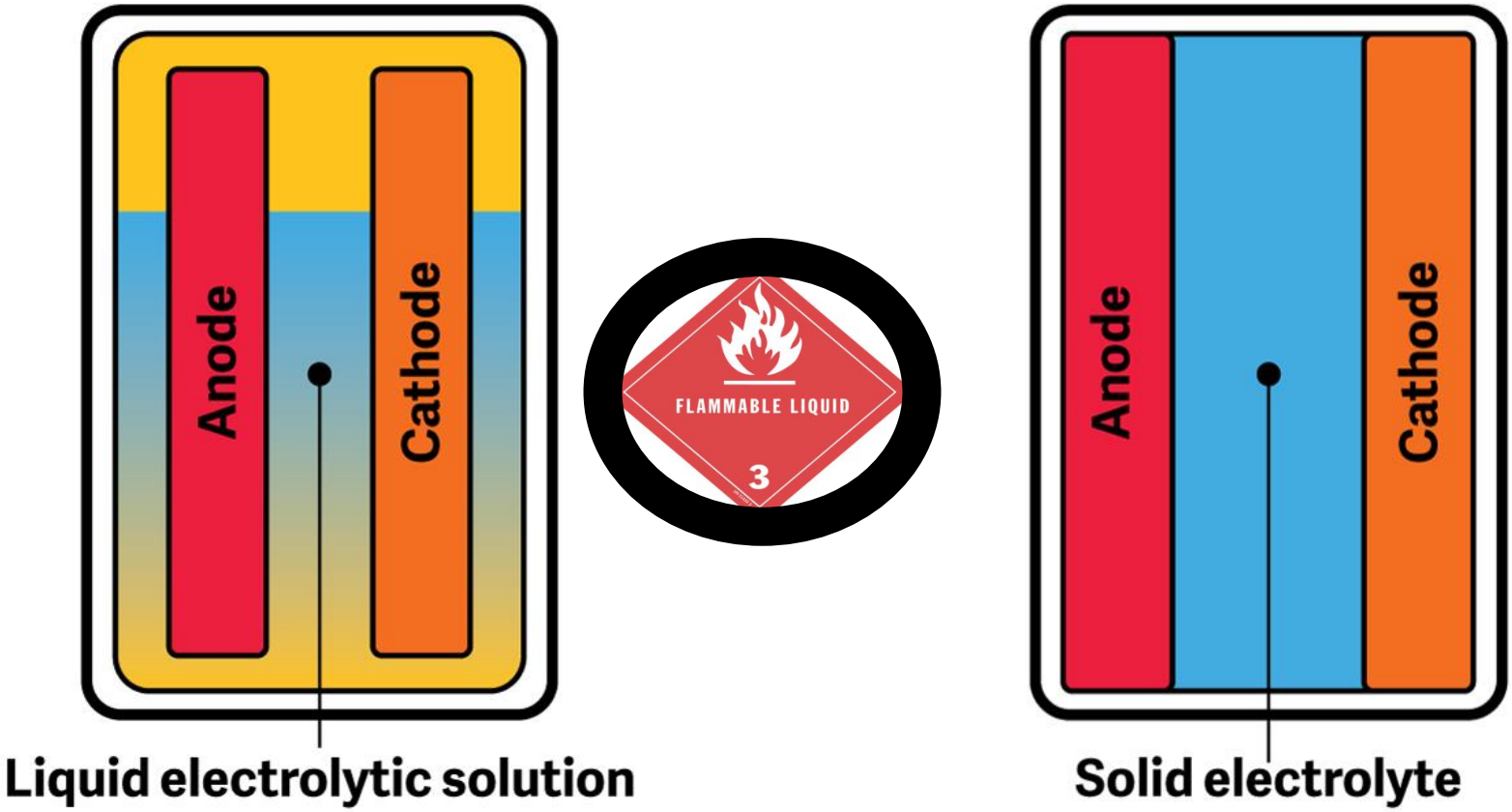
nature energy

House/Bruce (Oxford)

Future Outlook?

Beyond Lithium-Ion

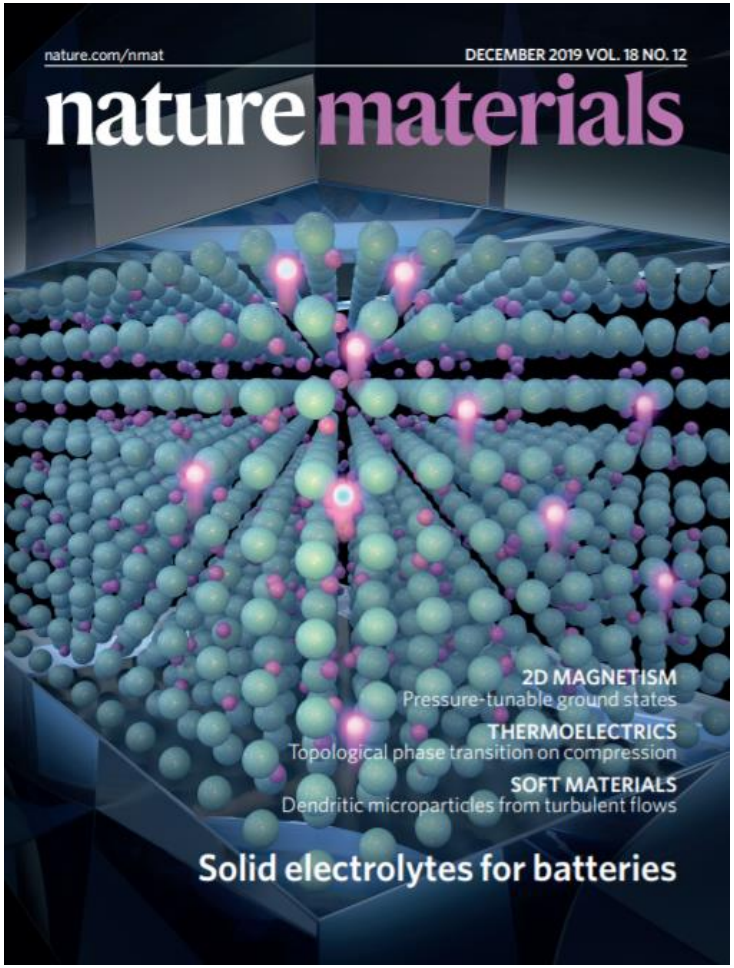
All Solid State



Safety, stability, high energy density (Li anode)

Mauro Pasta, Oxford

Review on Solid Electrolytes



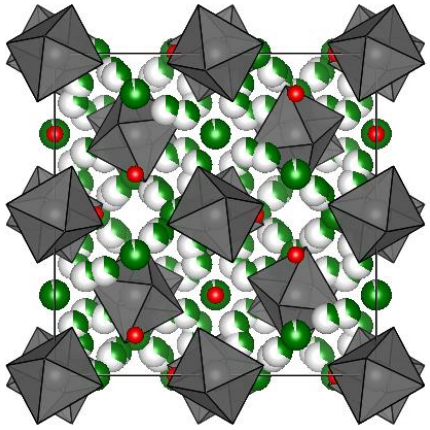
nature materials
REVIEW ARTICLE
https://doi.org/10.1038/s41563-019-0431-3

Fundamentals of inorganic solid-state electrolytes for batteries

Theodosios Famprikis[1,2,3*], Pieremanuele Canepa[2,3,5], James A. Dawson[2,3], M. Saiful Islam[2,3*] and Christian Masquelier[1,3,4*]

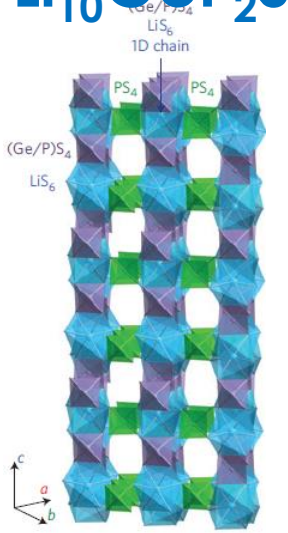
Garnet oxides

$Li_7La_3Zr_2O_{12}$



Sulphides

$Li_{10}GeP_2S_{12}$



Sodium-Ion Batteries

- Lithium resources
- Sodium: abundant & low cost
- Storage for grid
- New materials chemistry

Concluding Remarks

Battery Pipeline & Oxford Projects

Raw materials

Battery materials

Electrodes + components

Cells

Modules + packs

Vehicle applications

2nd life + recycling

Projects led by Oxford Materials

Cathode materials - CATMAT (S. Islam)

Solid state batteries - SOLBAT (P. Bruce)

Electrode manufacturing - NEXTRODE (P. Grant)

THE FARADAY INSTITUTION

EPSRC
Engineering and Physical Sciences Research Council

Take Home Messages

Challenge: CO_2 emissions & air pollution from road transport

Growth: lithium batteries & electric vehicles

Need advances in batteries: energy density, cost, safety

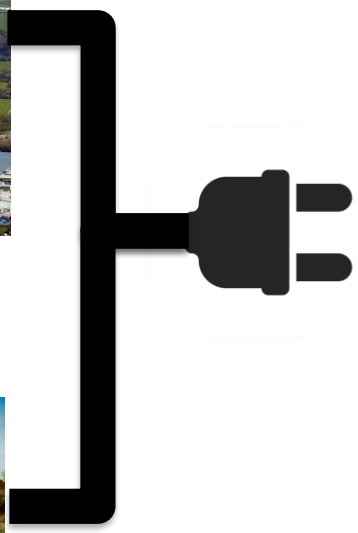
Innovation: sustainable materials, new battery science, recycling

The **End**

Possible…

Electricity & Low Carbon Energy

EVs are only as clean as the energy used to charge them…



Zero Emission

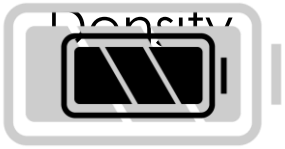
Battery Roadmap – 15-20 year timescale

Cost

Now $130/kWh (cell) $280/kWh (pack)

2035 $50/kWh (cell) $100/kWh (pack)

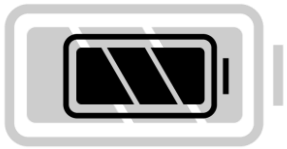
Energy Density



Now 700Wh/l, 250Wh/kg (cell)

2035 1400Wh/l, 500Wh/kg (cell)

Power Density



Now 3 kW/kg (pack)

2035 12 kW/kg (pack)

Safety

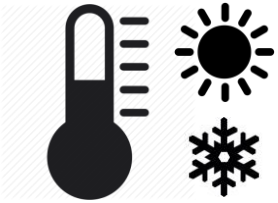
2035 eliminate thermal runaway at pack level to reduce pack complexity

1st Life

Now 8 years (pack)

2035 15 years (pack)

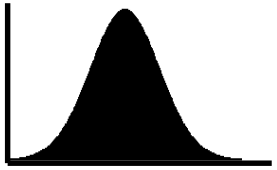
Temperature



Now -20° to +60°C (cell)

2035 -40° to +80°C (cell)

Predictability



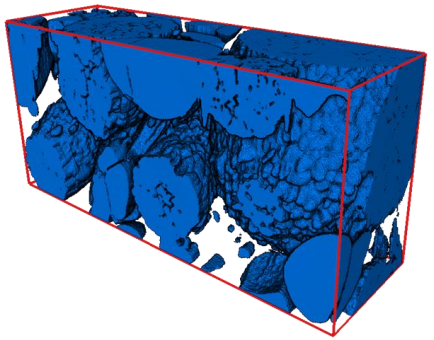
2035 full predictive models for performance and aging of battery

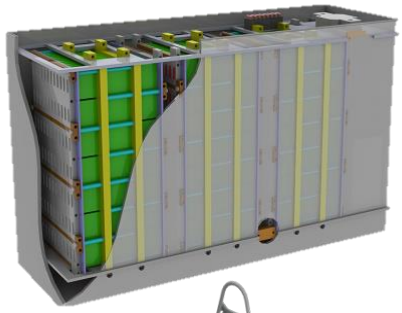
Recyclability

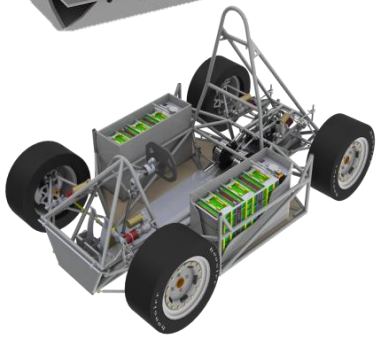
Now 10-50% (pack)

2035 95% (pack)

Are we there yet?







- **Rapid growth in battery cell manufacturing undeniable**
- **Race to develop battery manufacturing supply chains**
- **Nickel-rich NMC/NCA still dominant chemistry but with growing LFP market share**
- **Increasing concern over nickel and lithium availability**
- **Fast charging issues starting to be addressed**
- **Overcoming manufacturing challenges are critical for success**
- **Increasing interest in lithium metal anodes**
- **Solid-state battery developments have rapidly advanced**
  - **Sulfides, oxides and polymers**
- **Lifetime and supply chains limits rate of innovation**
- **Recycling emerging but economics still challenging**

Quick Aside:
Alternative Battery!

BBC TV Christmas Lectures 2016

Guinness World Record = 1,275 V

RSC Team in October 2021

Guinness World Record = 2,304 V

Used lemons processed by Refood to biogas

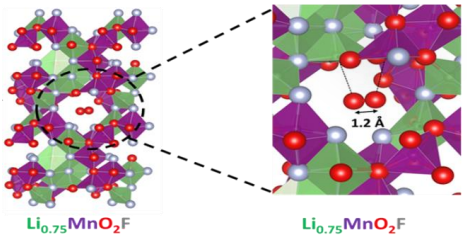
Unlikely…

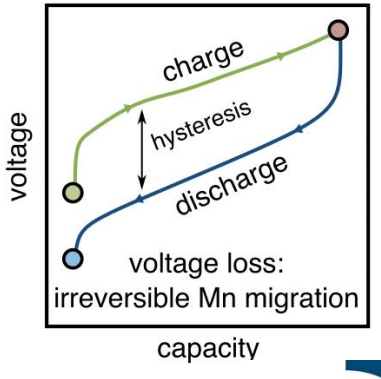
Design rules: Disordered rocksalts (bath/OXF)

- **AIM: Understand and prevent hysteresis in Mn-based disordered rocksalt cathodes to retain voltage during cycling**

- **OUTPUT/SUCCESS: Identified mechanism for O_2 formation (*JACS, 2020*) & hysteresis and proposed design rules for improved performance: (*EES, in review*)**

- **NEXT STEPS: Study cathodes with varying composition, minimising Mn migration. Experimental (Oxf) guided by computational insights (Bath)**

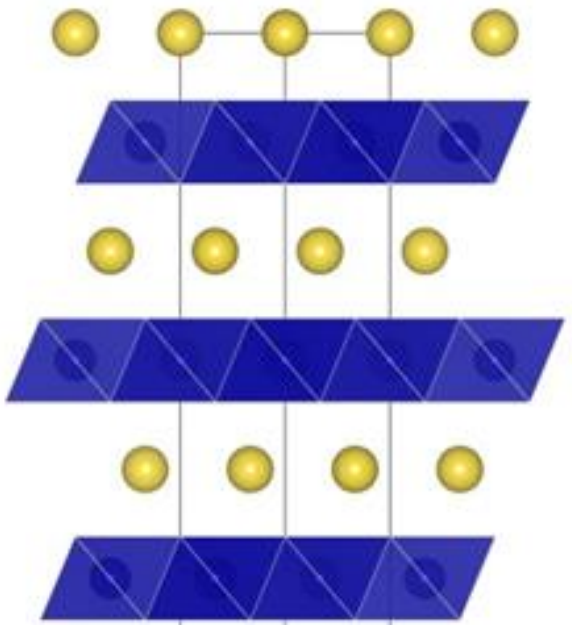




JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Energy & Environmental Science

Current Layered Cathodes

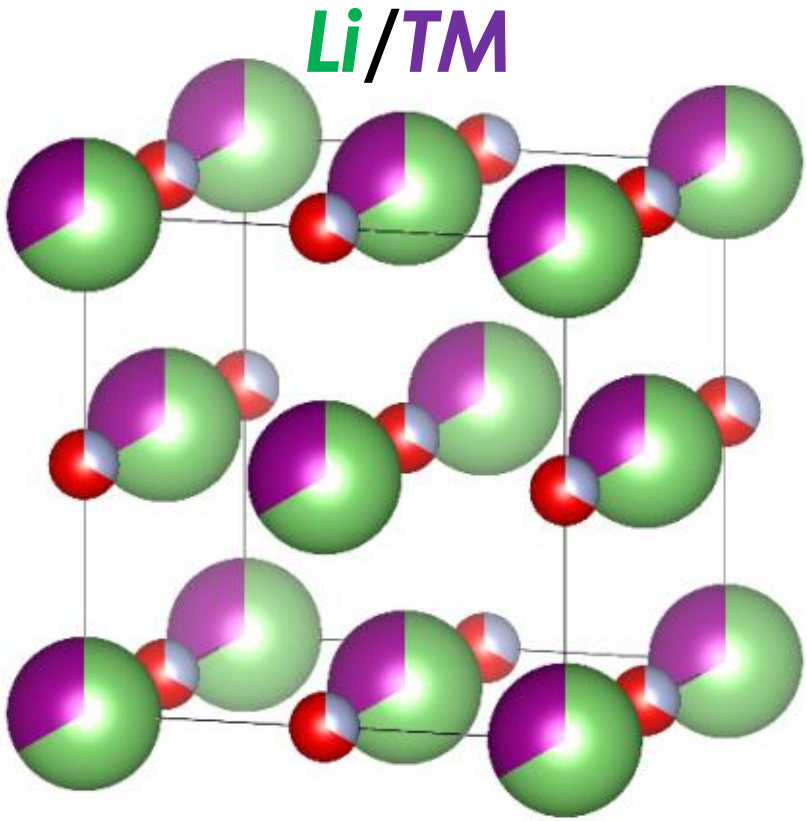


	Li	Li	Li
	Co	Ni,Mn,Co	Li,Ni,Mn
		'NMC-622'	*'Li-rich'*
mAh/g	140	180	250

- Conventional: store charge on transition metal
  - Li-rich: Li/TM > 1 → TM AND O redox
  - BUT problems (voltage fade, O2 loss)

Disordered Rocksalt Cathodes

- Li-rich: Li/TM > 1
- Li/TM disorder
- Capacity: 250-320 mAh/g
- Moving away from Co



Materials Science is Critical

Breakthroughs? New materials, new concepts & underpinning science

Green Light for Electric Cars

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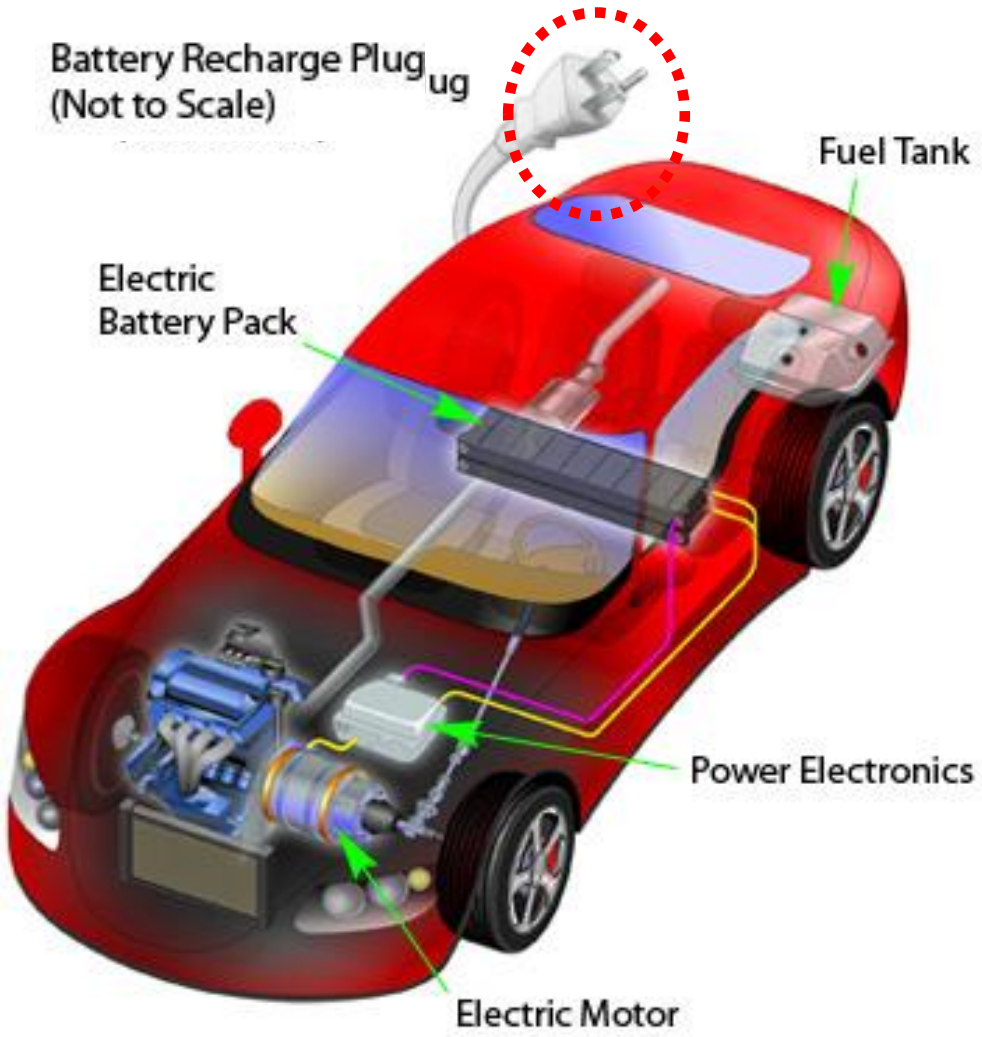
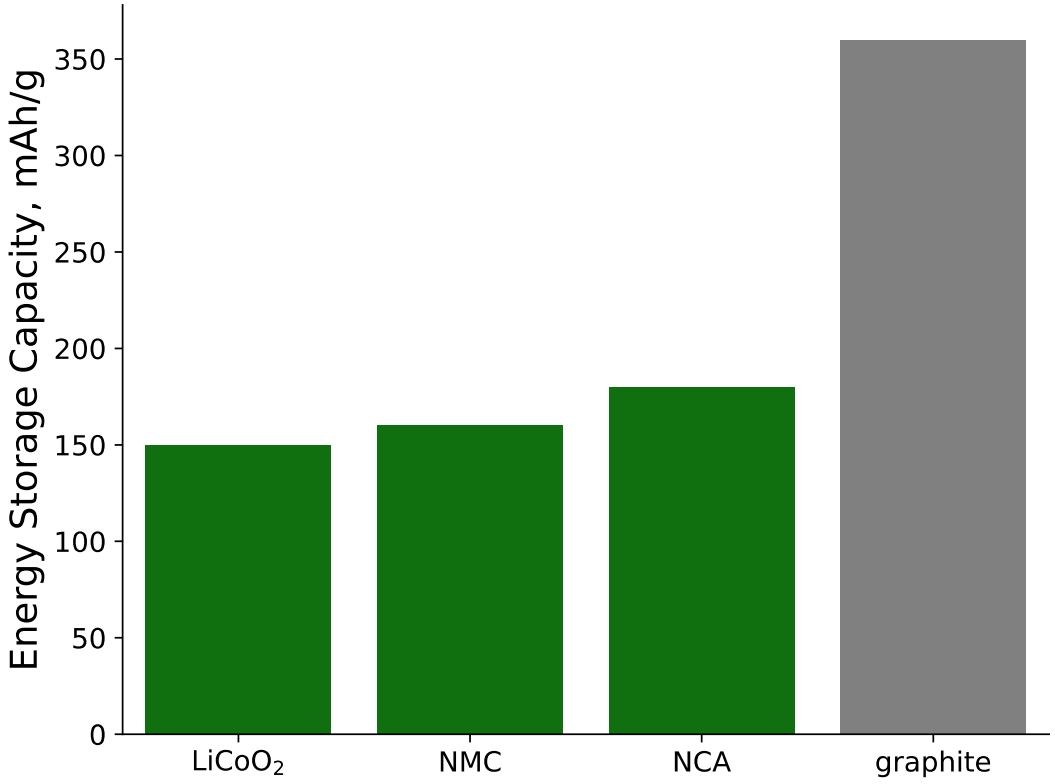
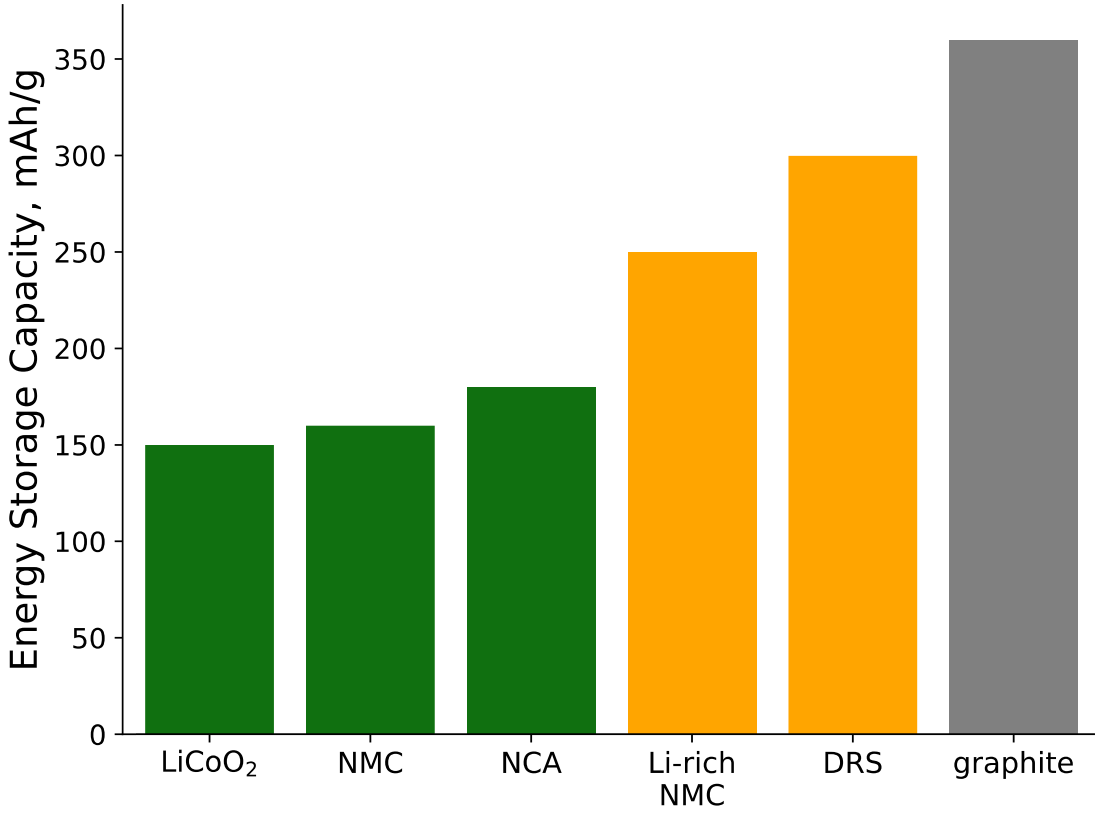
Science & Environment

Ban on new petrol and diesel cars in UK from 2030 under PM's green plan




Energy Storage Capacity, mAh/g
0
50
100
150
200
250
300
350
LiCoO2
NMC
NCA
graphite


Energy Storage Capacity, mAh/g
0
50
100
150
200
250
300
350
LiCoO2
NMC
NCA
Li-rich NMC
DRS
graphite

Energy Storage & an Electrified Future

Consumer electronics
Wh scale

Electric vehicles
kWh scale

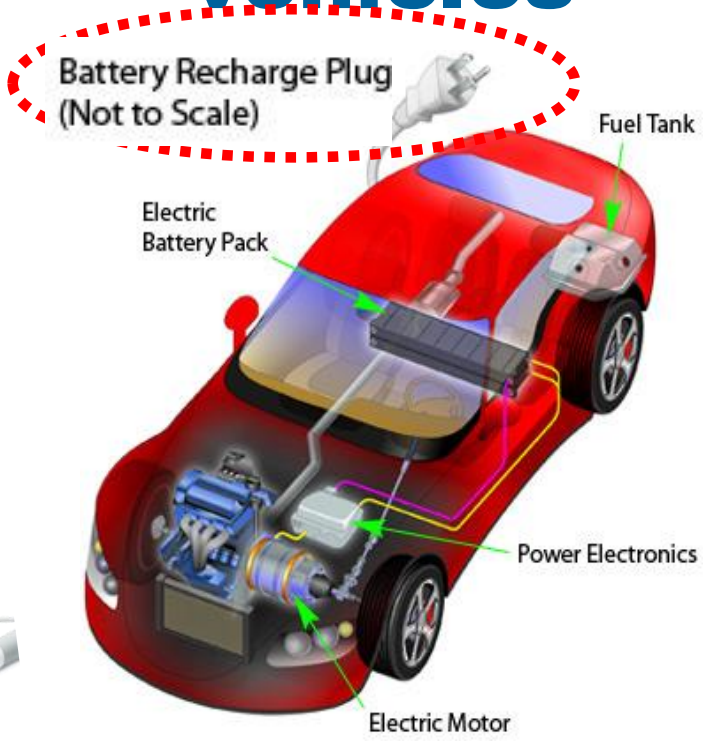
Balancing renewables
MWh scale

Add text? Lithium battery market > $150B

Energy Storage: Batteries

Portable revolution

Electric vehicles

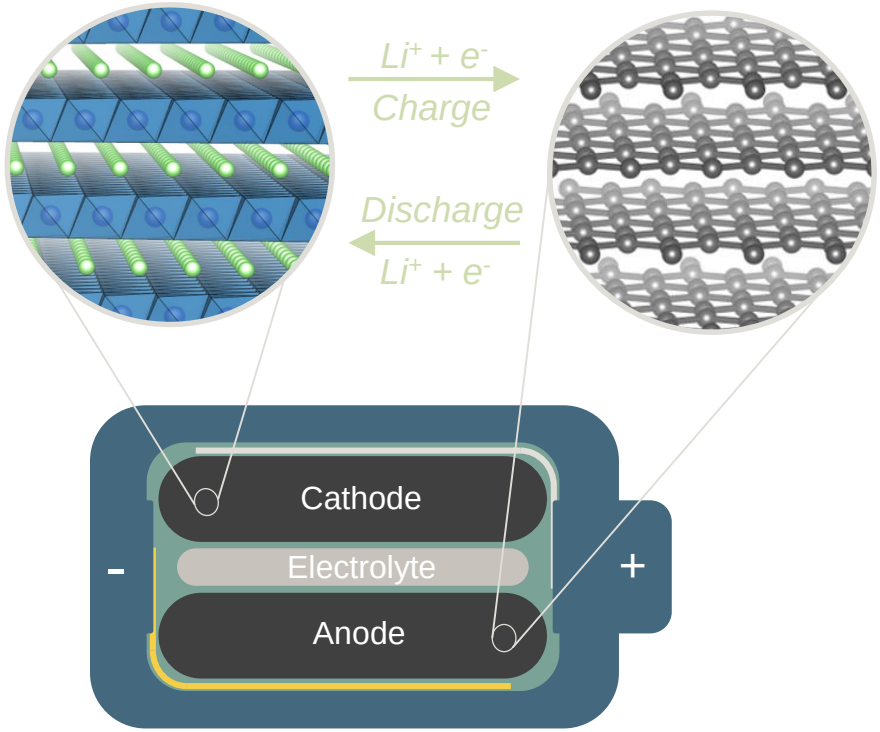


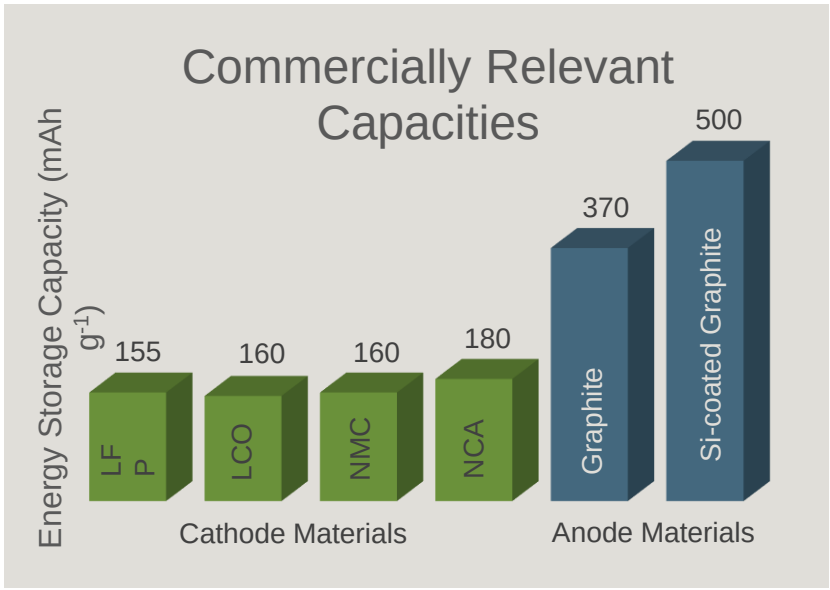
Grid storage

Step change advances?

Need New Cathode Materials

Cathode (oxide) vs Anode (graphite)





Current Li ion batteries

Approaching the practical limit for Li ion

State of the art

Specific energy 250 Wh kg^{-1}

Energy density 600 Wh l^{-1}

Range anxiety

$120/kWh

Target

300 mile range

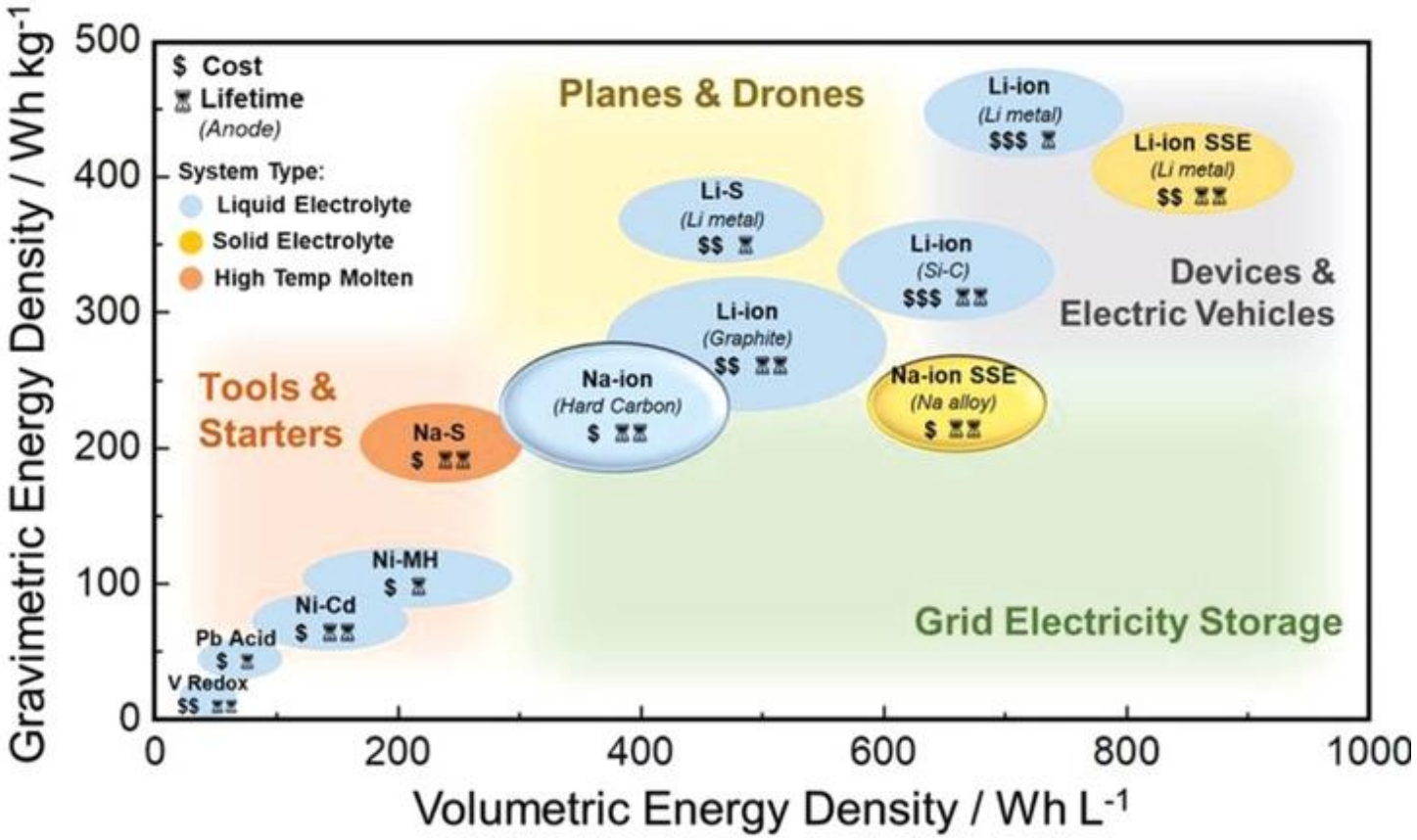
15 minute charge

< $100 /kWh

STEP CHANGE IS NEEDED

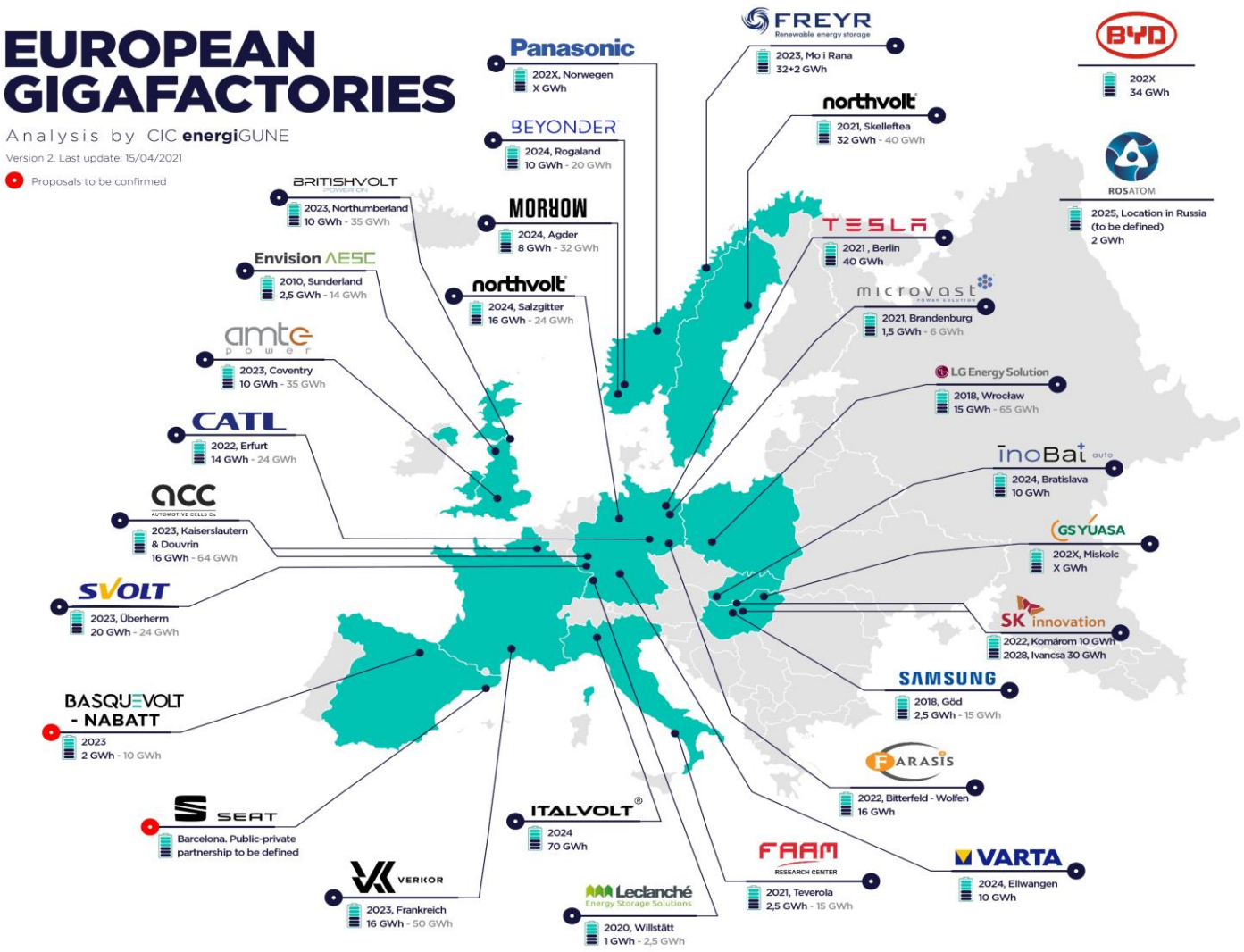
New knowledge, new science and new materials

BATTERY TECHNOLOGY APPLICATIONS

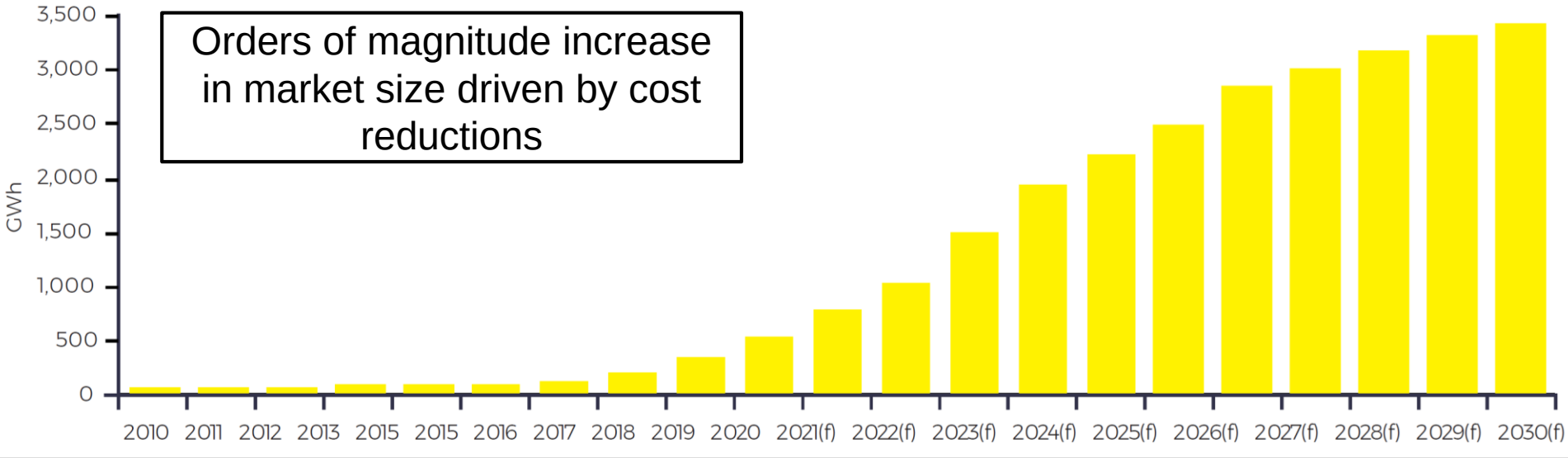


Adv. Energy Mater. 2020, 10, 2001274

Batteries in Europe?



Global lithium-ion battery megafactory capacity



Benchmark mineral intelligence March 2021

Batteries in Europe

Doctorate Programme on Emerging Battery Storage Technologies INspiring Young scientists

Marie Skłodowska-Curie actions COFUND PhD

Why power electric cars with lithium batteries

Highly efficient vs fuel cells

energy out : energy in

Li-ion ~ 90%,

Hydrogen ~ 40%

Much lower cost than hydrogen and fu

Potential for advancement delivering longer driving range and faster charging

We have an electricity infrastructure already

They work

Store more energy per unit mass and volume than other batteries

Main Challenges- Current State and Step Change Goals

225 Wh/kg	Cycle life 1500-2000
Calendar life ~5-7 years	Cost >£100/kWh
>300 Wh/kg	<£100/kWh
> 10 years	

DOES NOT DELIVER THE PERFORMANCE AT COST REQUIRED FOR FUTURE Evs AND GRID SCALE STORAGE

Batteriernas livslängd – är det ens ett problem?

Hur många år och laddningar? 10 år & 1 laddning per dag?

Hur mycket *sämre* batteri är OK? 10%?

OK?! $90\% = (\eta)^{4000} \Rightarrow \eta = 0{,}999975 = 99{,}9975\%$

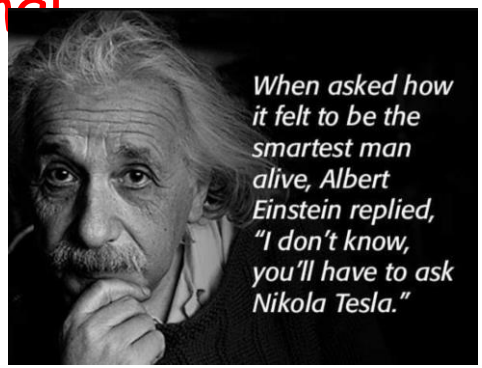
e batteri per laddning!

m!

Teslas "Million miles battery"?

370 miles/laddning x 4000

=> 1.500.000 miles = OK!



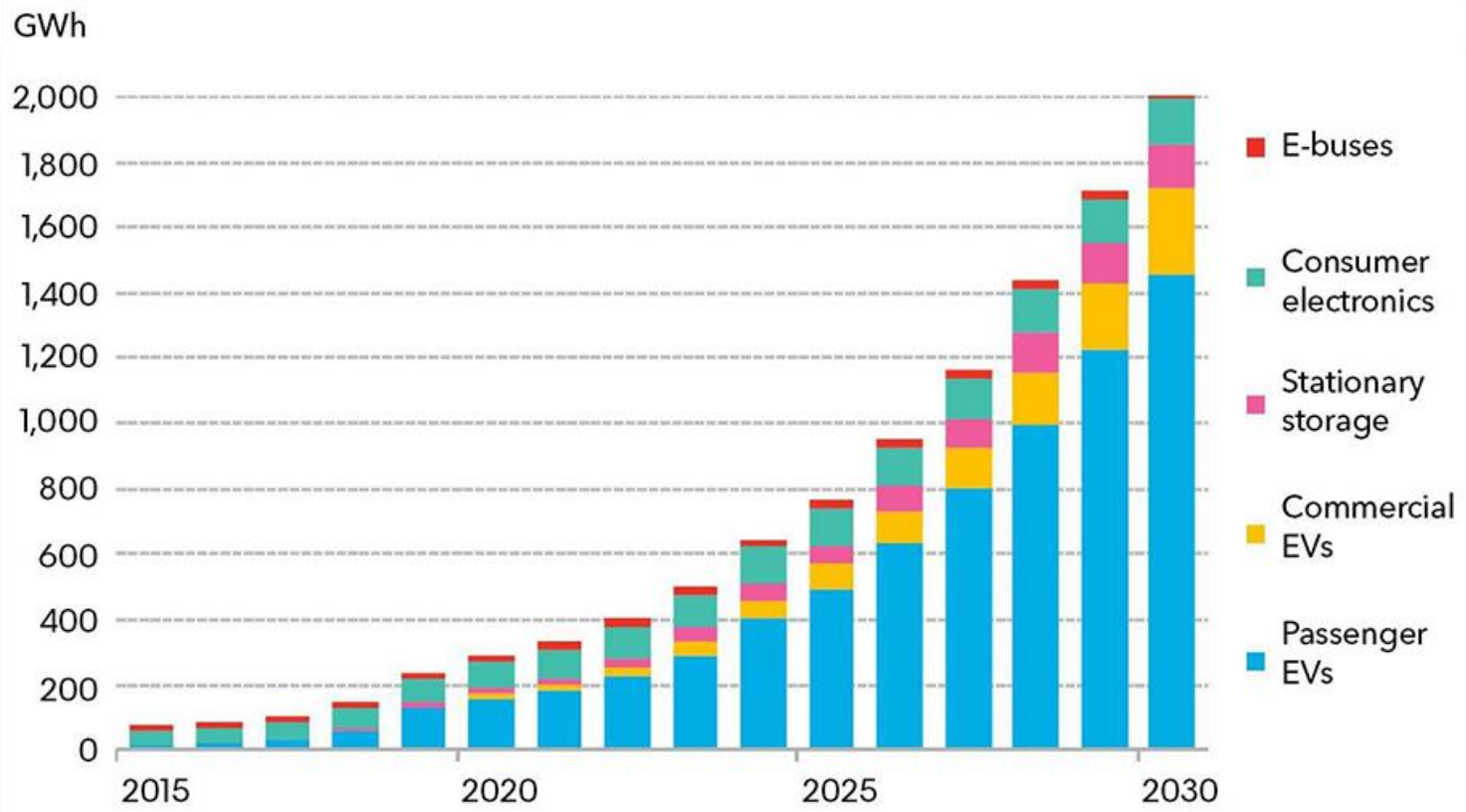
Inevitable transition to electric vehicles

Country	Proposed phase out date/status
Canada	2040
China	Researching timetable
France	2040
Iceland	2030
Netherlands	2030
Norway	2025
Singapore	2040
Sweden	2030
UK	2035

Lithium battery market $150B by 2030

Global Li-ion Battery Market

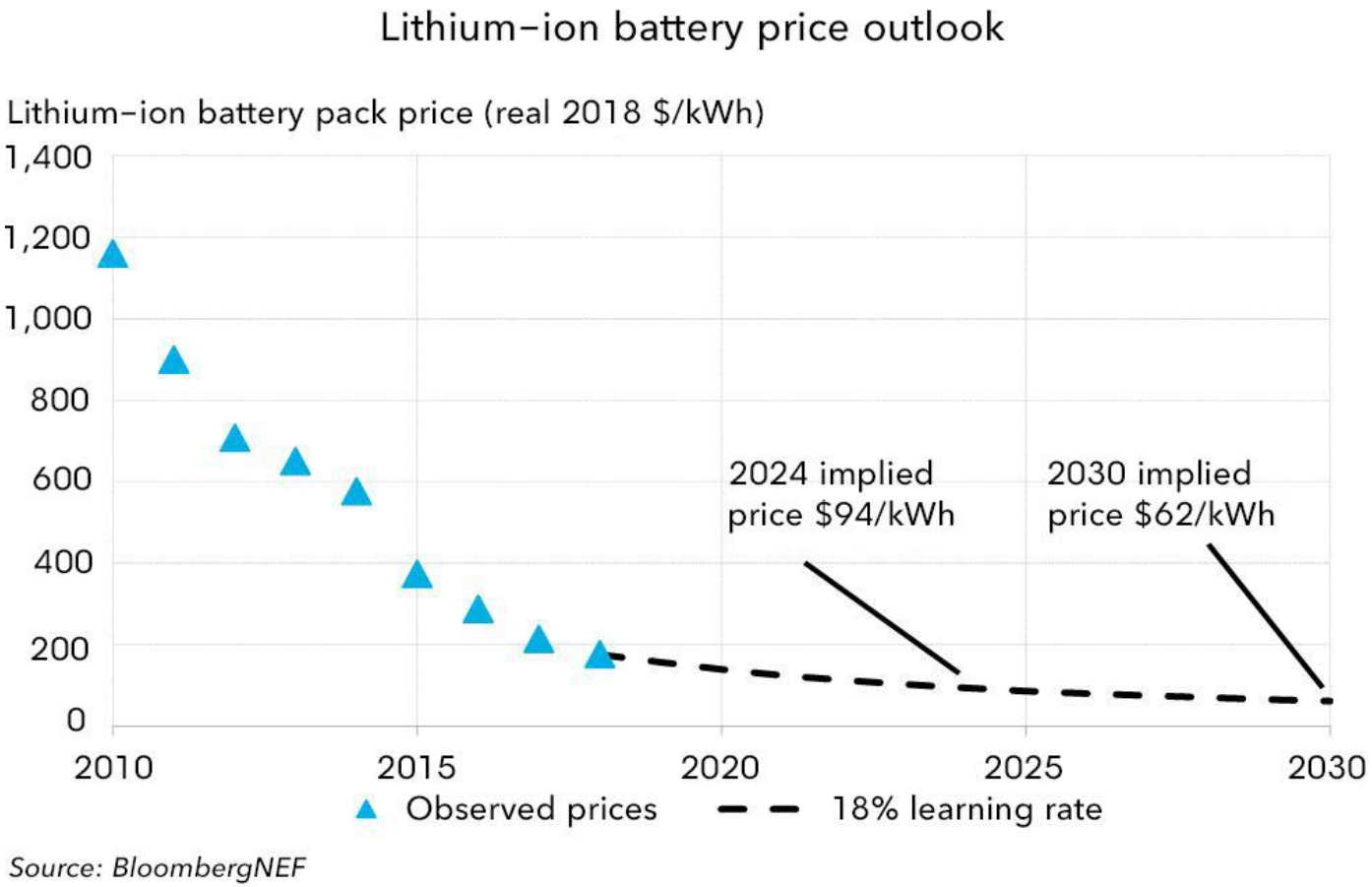
- Rapid market growth predicted
- Driven by the transition from ICE to EV



Source: BloombergNEF, Avicenne

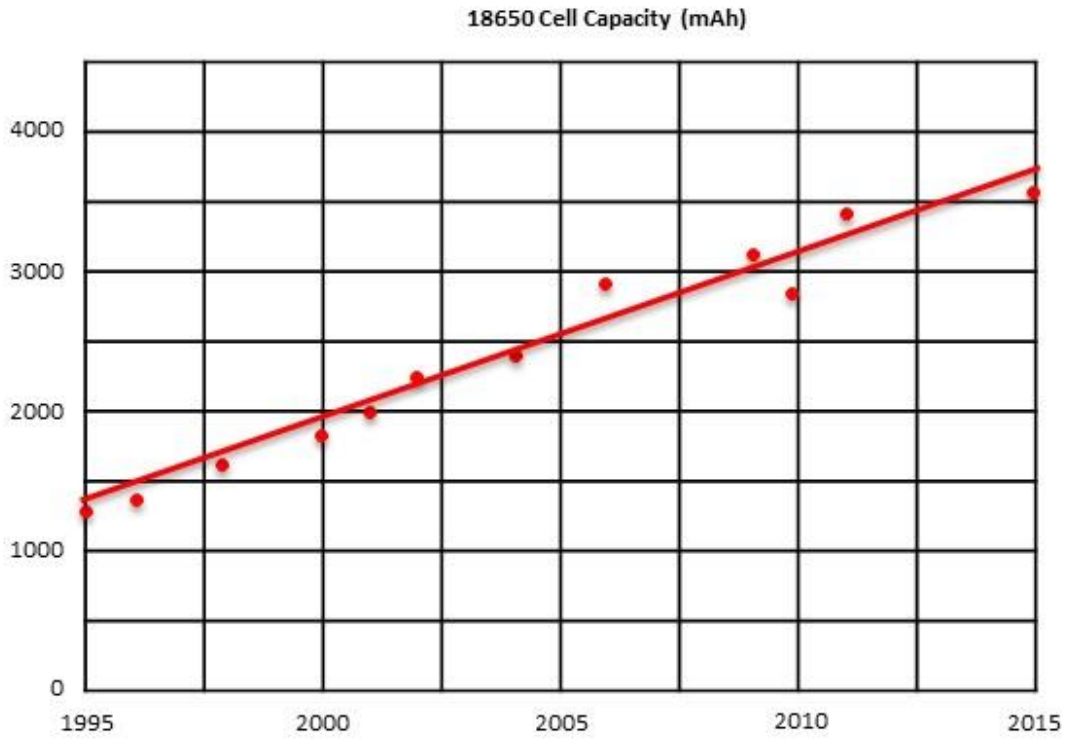
LI ION PACK PRICES

- Rapid fall in price over the last decade
- Prices expected to continue falling but at a lower rate



Source: BloombergNEF

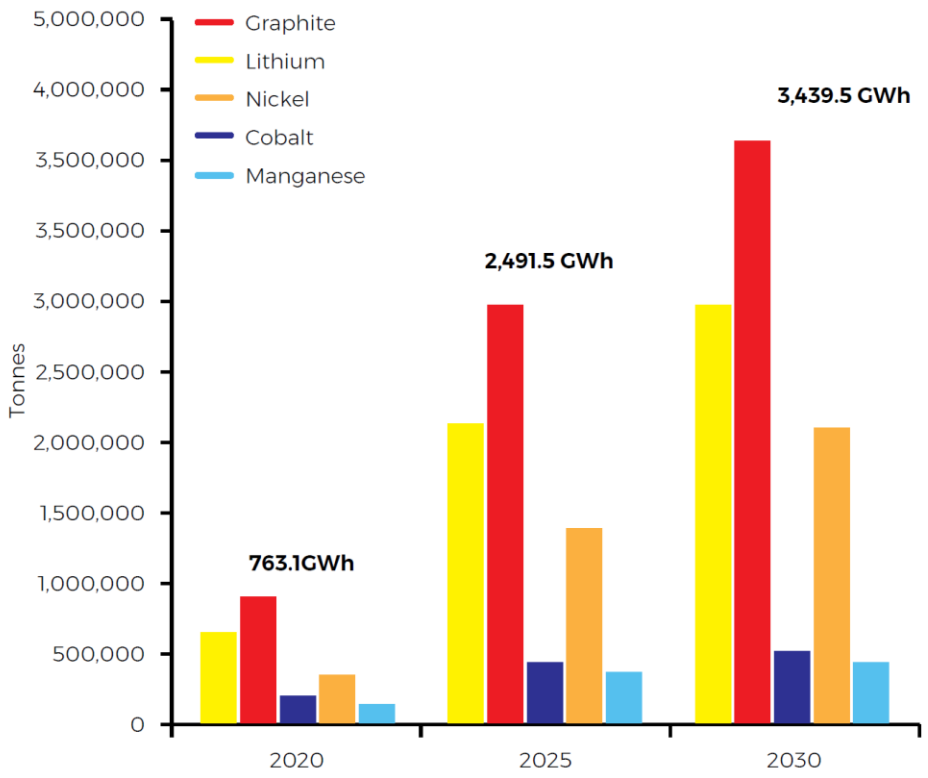
Batteries: Cost & Energy Density



- Volumetric energy density is increasing due to better materials and cell structure
- Doubled in 15 years
- Requires continued innovation to continue

Nykvist et al 2014

Impact on raw materials

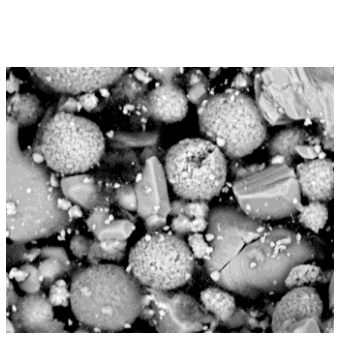


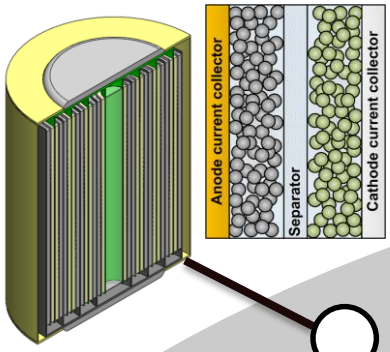
Benchmark mineral intelligence March 2021

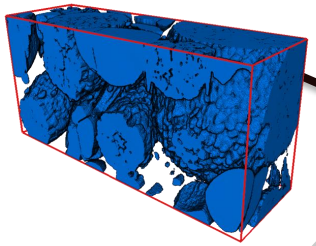
MATERIAL	2020	2025	2030
LITHIUM	648,000	2,143,000	2,990,000
GRAPHITE ANODE	906,000	2,990,000	4,163,000
COBALT	195,000	433,000	516,000
NICKEL	343,000	1,392,000	2,113,000
MANGANESE	135,000	366,000	432,000
TOTAL GWh	755.1	2,491.5	3,439.5

Along with increasing capacity demand there is a shift to nickel rich/low cobalt cathodes and silicon/lithium-metal anodes

How do we make better batteries?





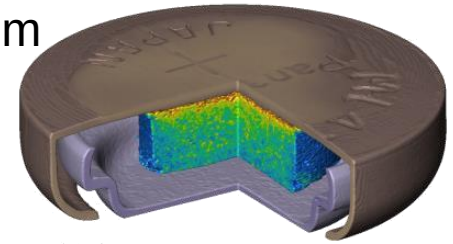


Microstructure

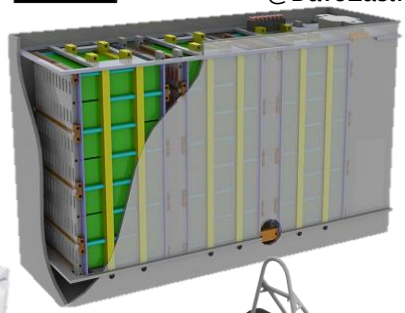
Cell design

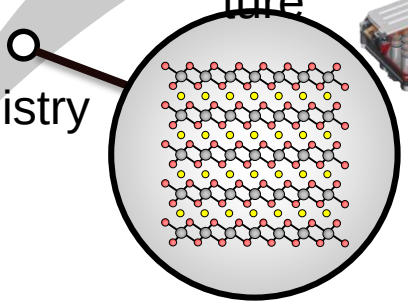
Pack design

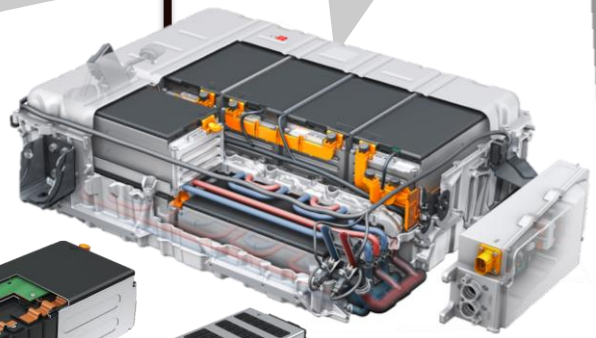
Multi-length scale problem



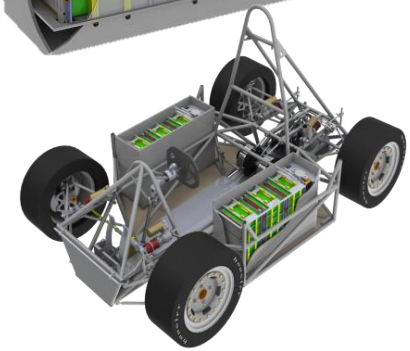
@DaveEastwood







@Audi



Chemistry

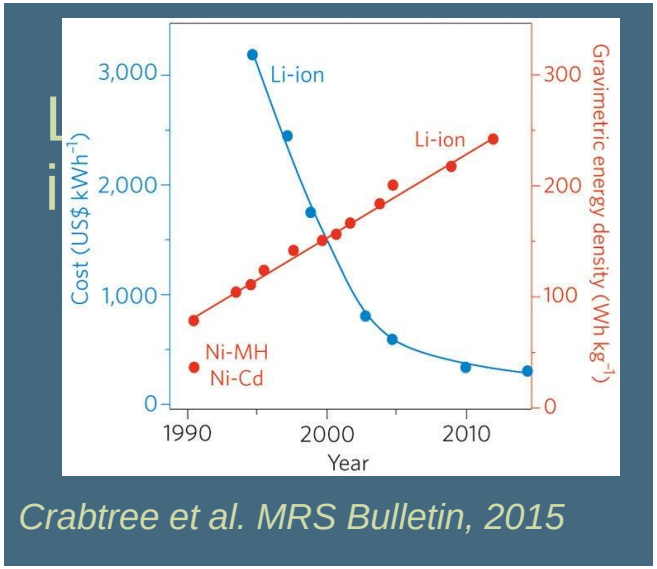
Energy Storage & an Electrified Future

Global Warming

Intermittent Renewables

Poor Air Quality

Portable Electronics



Crabtree et al. MRS Bulletin, 2015

Li-ion Diffusion: Charge Rates

-*Important for charging*

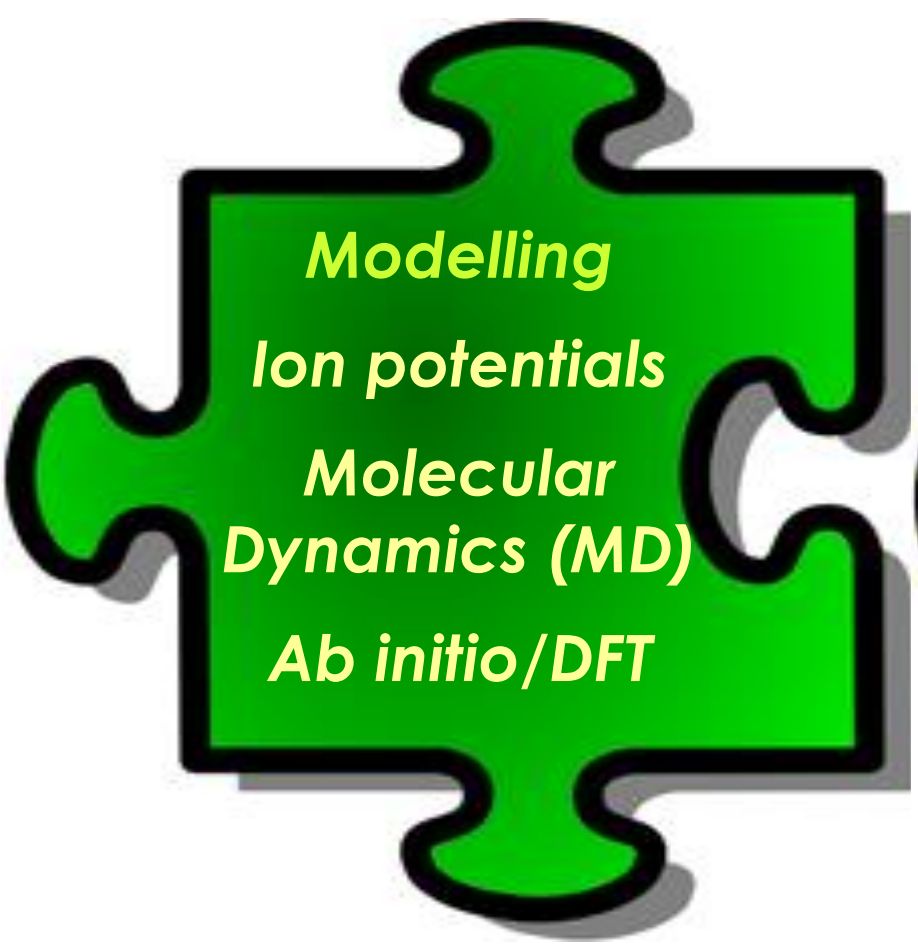
-*Fast* 1D, 2D, 3D pathways?

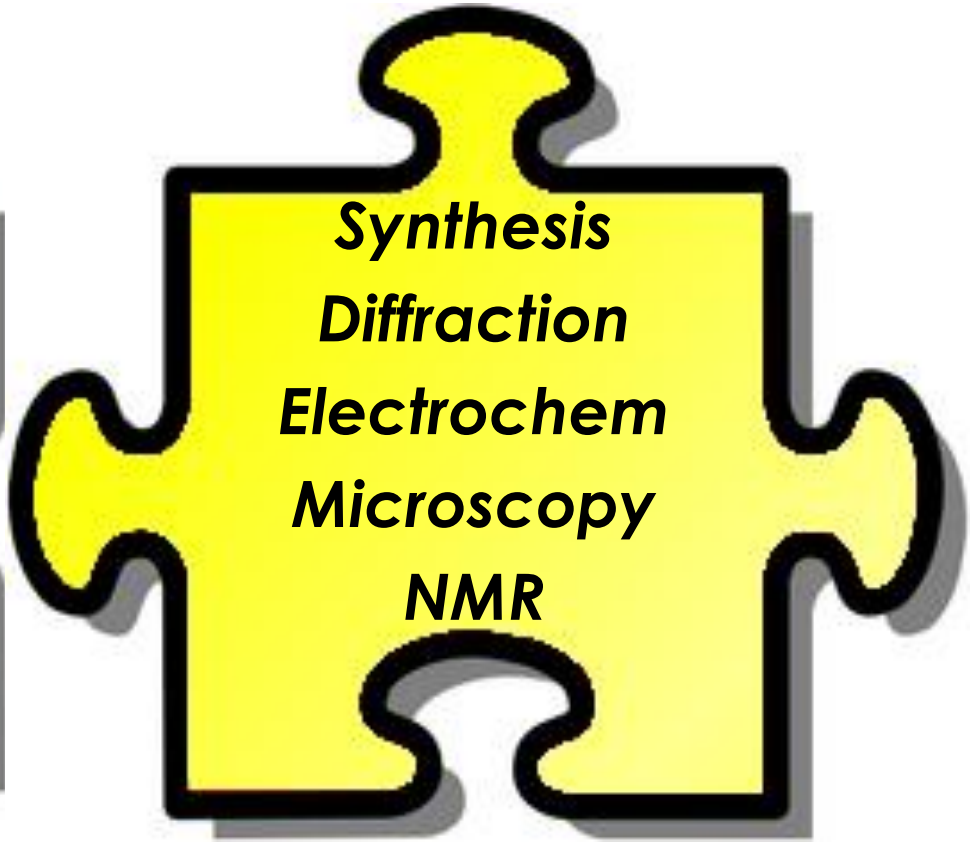
-New materials: *not fully understood*

$LiCoO_2$: Li-ion conduction

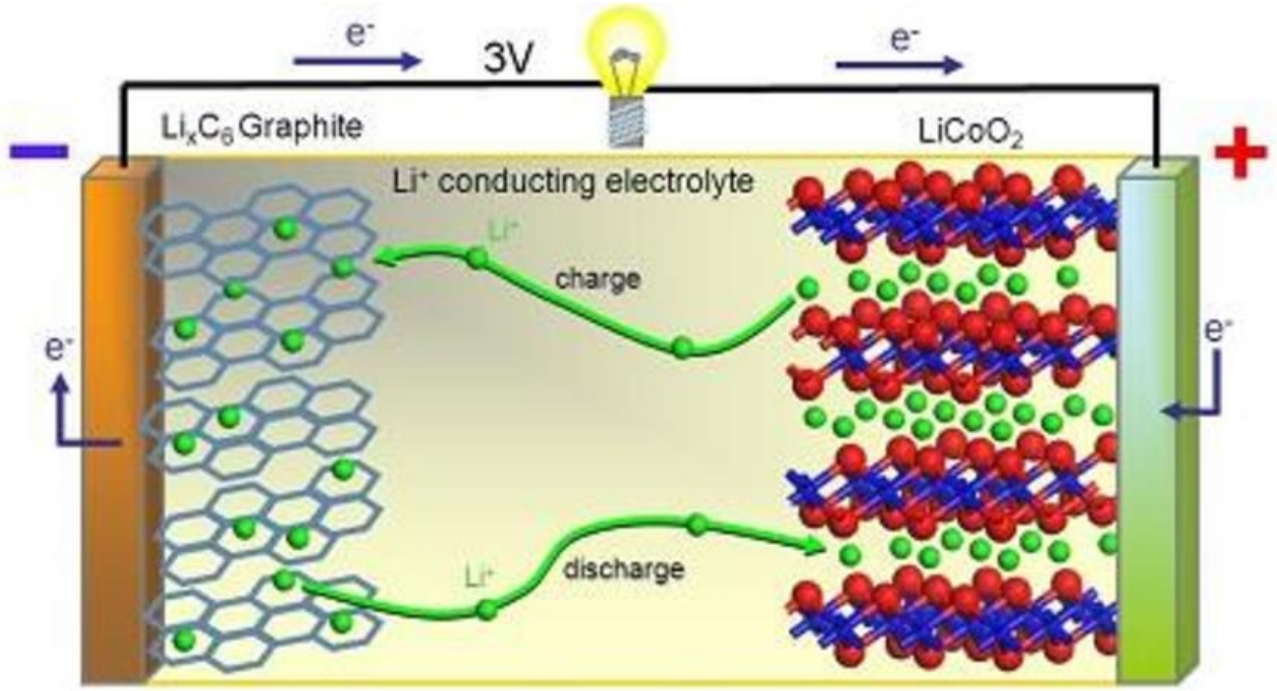
Emig ~ 0.4eV D(Li) ~ 10-9cm2/s

Modelling-Experimental Synergy





Lithium-Ion Battery



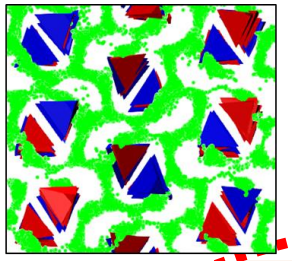
Graphite anode

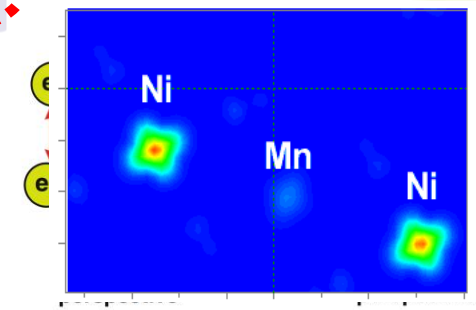
$LiMO_2$ cathode

New? Energy density, safety, cost, lifetime

Modelling Methods vs Scale

$$\phi_{ij}(r) = \left(\frac{q_i q_j}{r}\right) + \left(A_{ij}\exp\left(\frac{-r}{\rho_{ij}}\right)\right) - \frac{C_{ij}}{r^6}$$





Years

Femto

Time Scale

Continuum

Finite Element

Monte Carlo

Molecular Dynamics

Density Functional Theory

ab initio methods

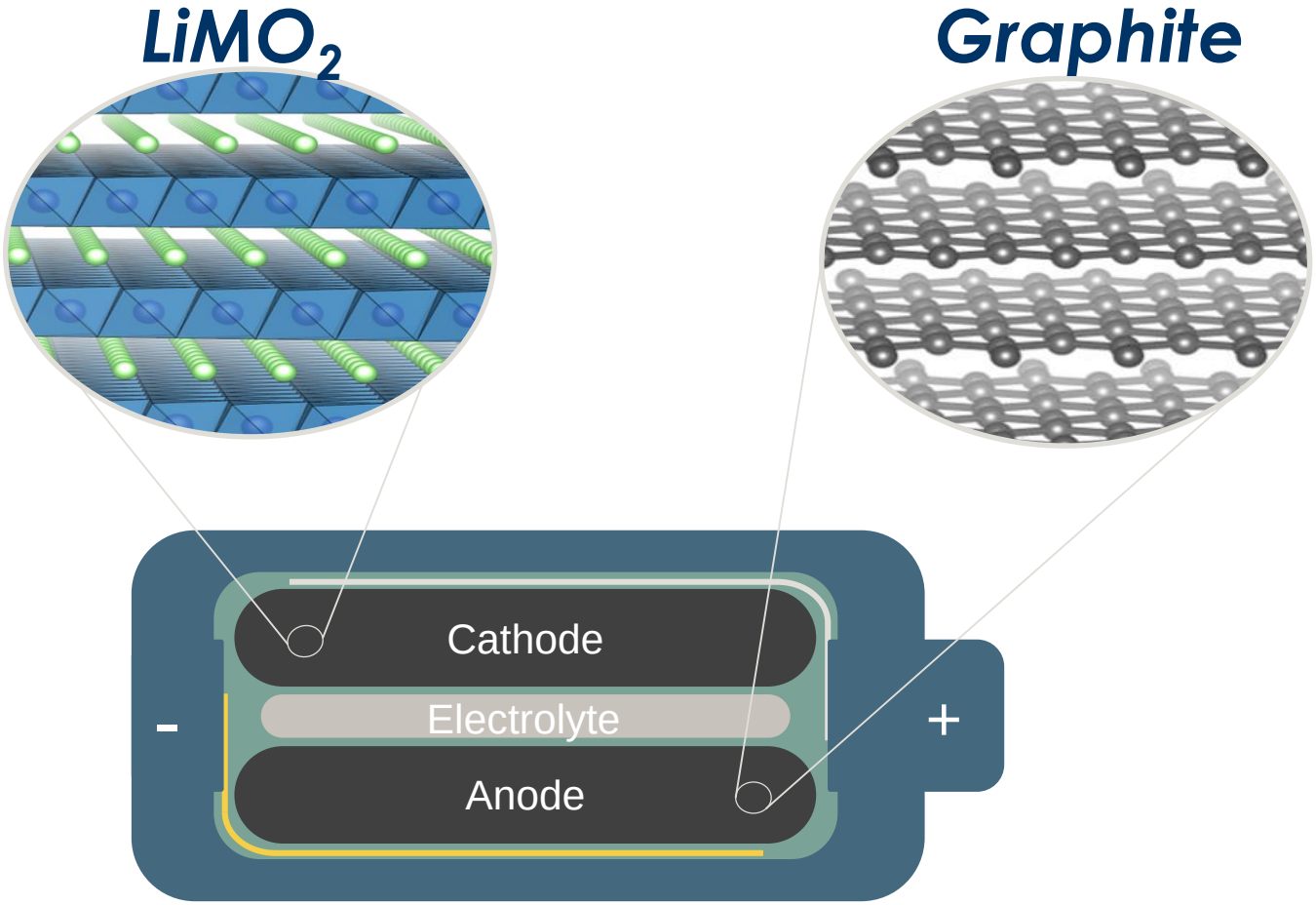
Ångström

Meters

Length Scale

Electrons | Ions | Grains | Films | Devices

Lithium-Ion Battery

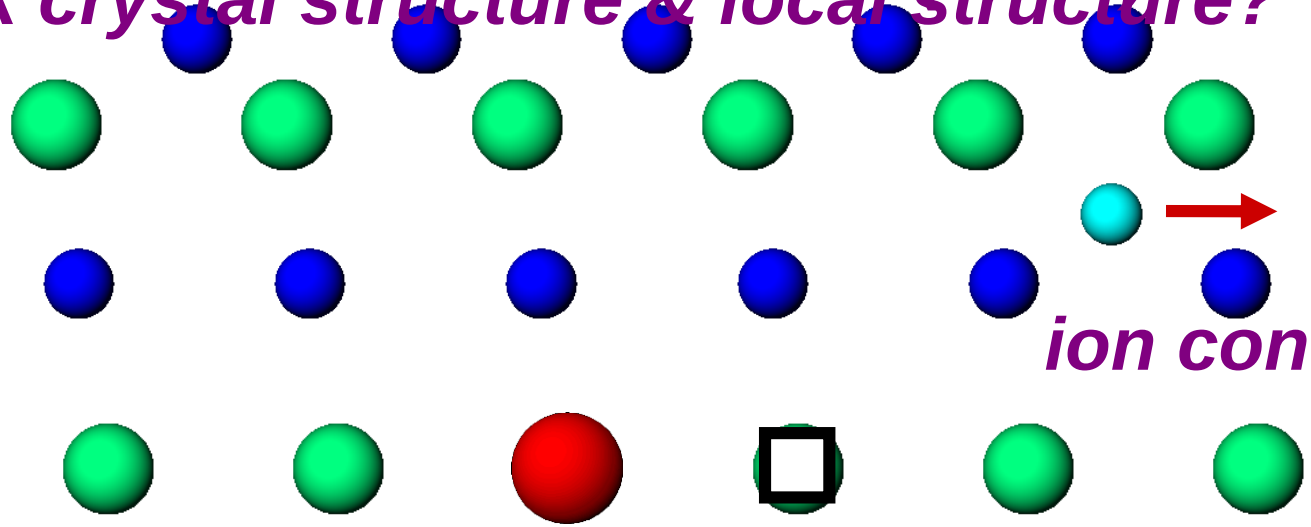


Materials Properties

Characterisation & deeper understanding

Surfaces & interfaces of (nano)materials?

Bulk crystal structure & local structure?



ion conduction?

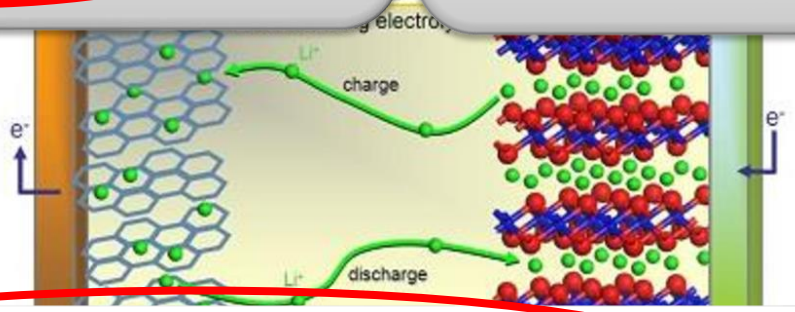
Doping & electronic behaviour?

Defects & disorder?

Battery Materials Research

Cathode
$Li(Ni,Mn,Co)_2$ NMC
Li-rich oxides

Anode
Lithium
Silicon

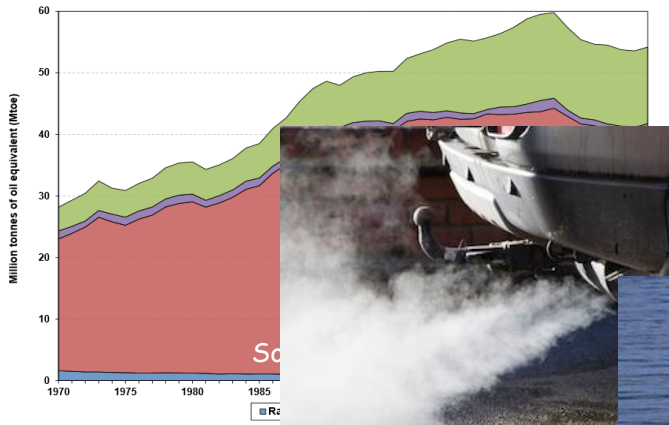


***Electrolyte*: solid-state, polymer**

***Beyond Li-ion*: Na+, Mg2+**

***Beyond Intercalation*: Li-S & $Li-O_2$**

Chart 2 Transport energy consumption by type of transport, UK (1970 to 2014)



Energy Demand

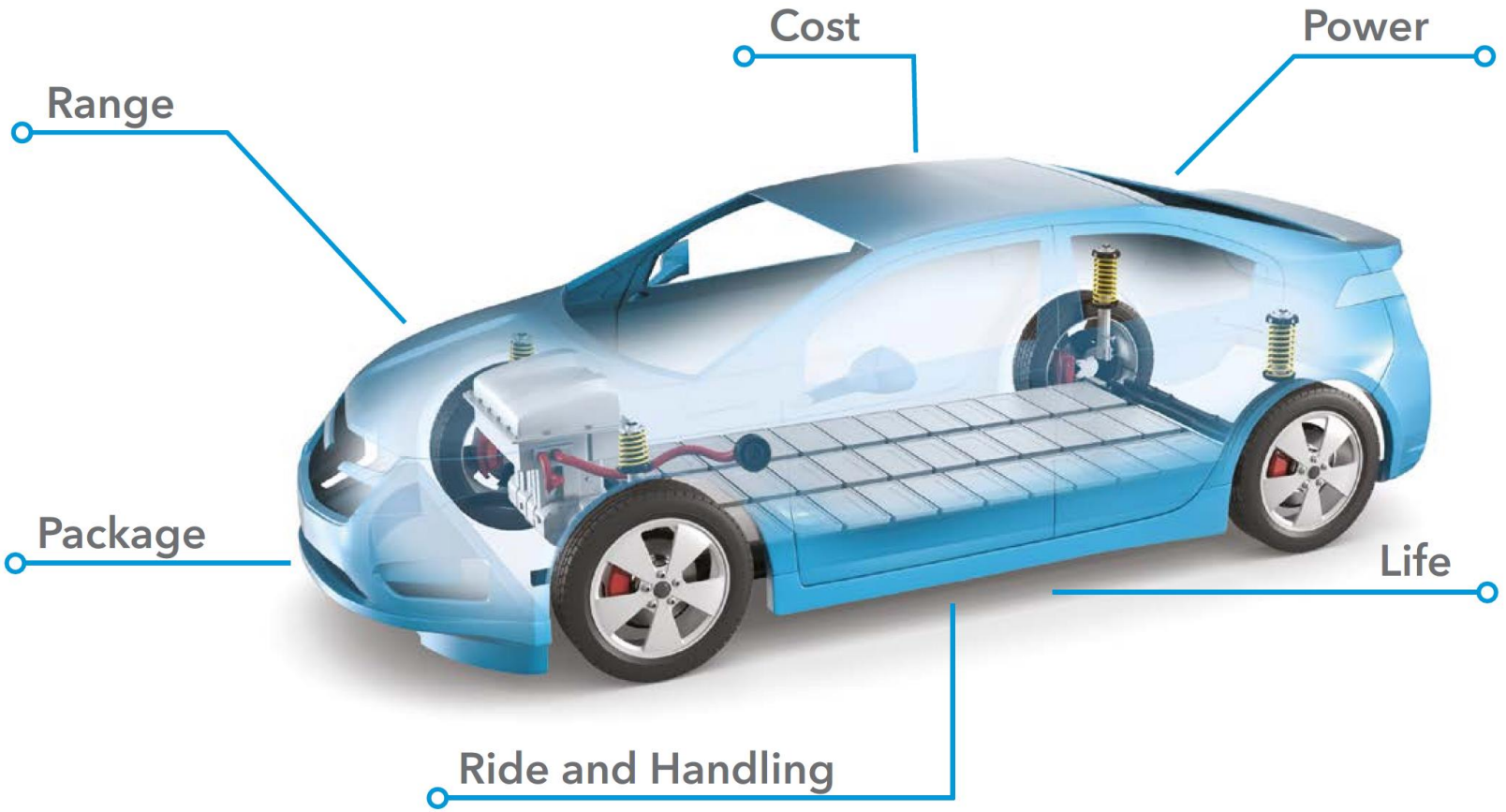
Air Quality

Climate Change

Congestion

Accidents

The battery is the defining component of the electric vehicle



Energy Storage & an Electrified Future

Global Warming

Intermittent Renewables

Poor Air Quality

Portable Electronics

Road Transport

What can we do about CO_2 emissions?

Manage Demand

- Travel Less


- Use best transport mode



- Manage transport network

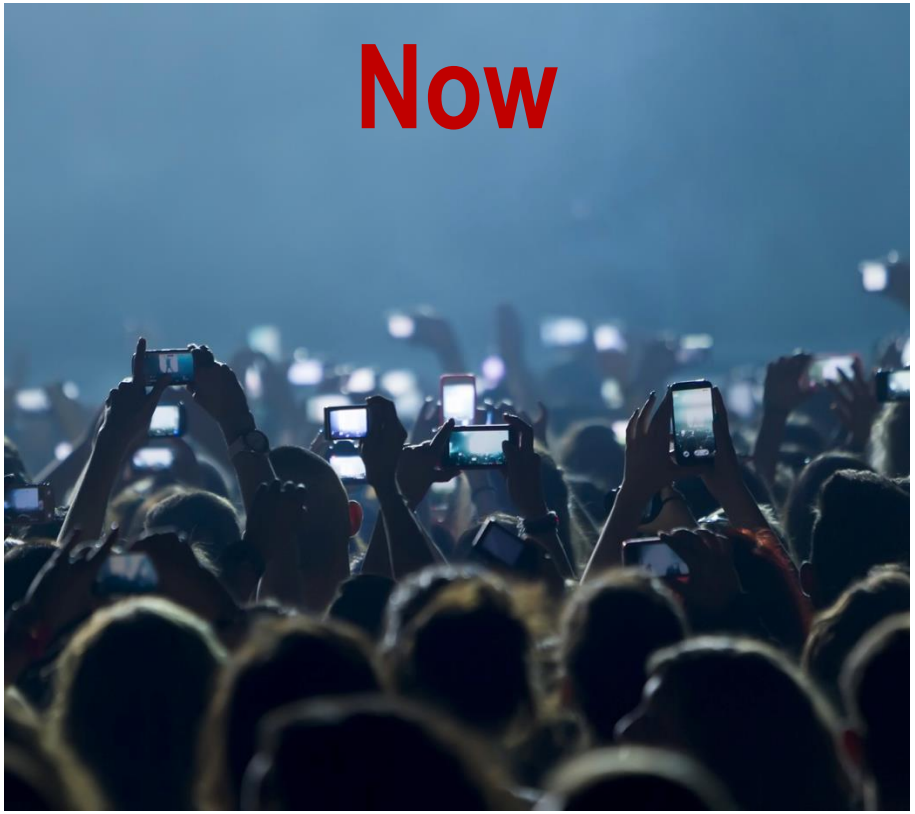

Improve Technology

- Reduce vehicle mass and drag

- Improve powertrain

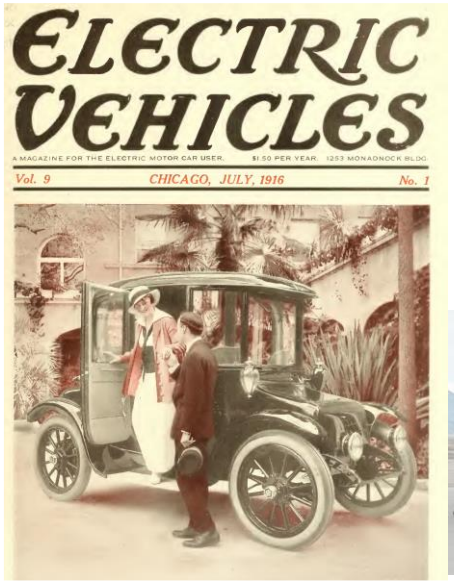
- Reduce carbon in fuel

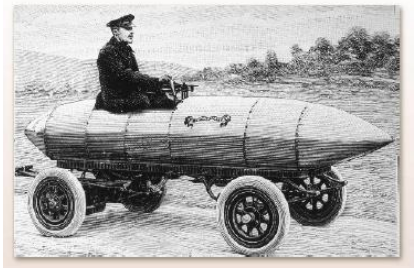
Portable Revolution

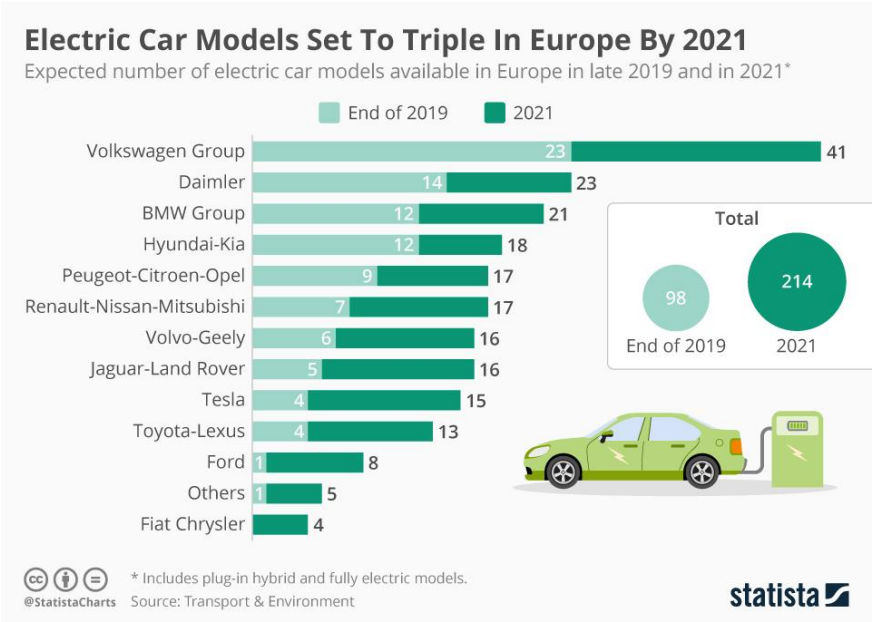


High energy density lithium-ion batteries

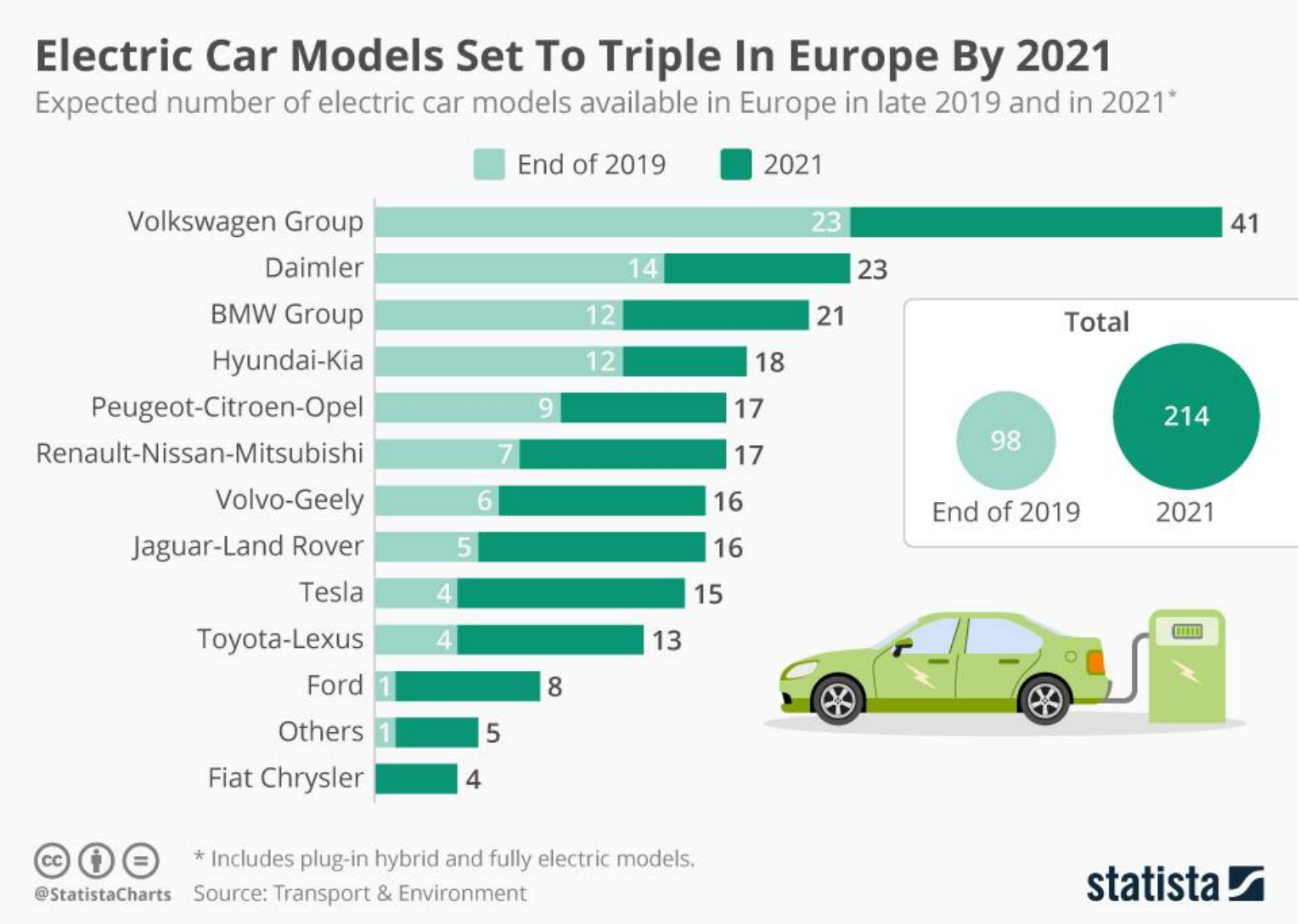
Electric Cars: Then & Now



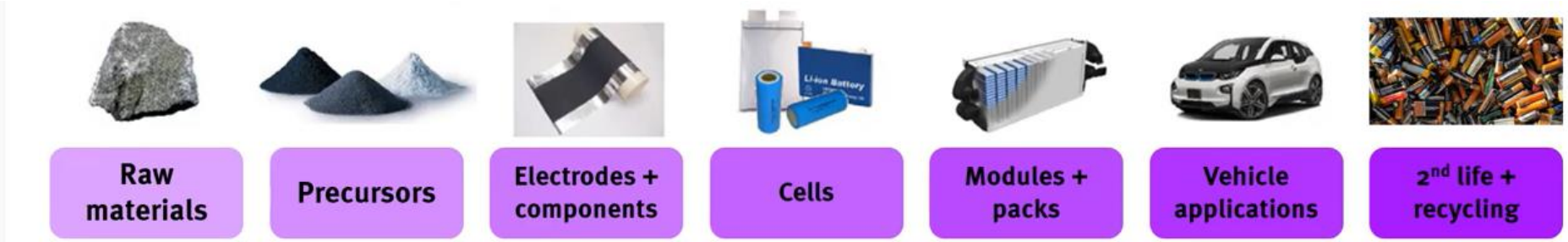




Electric Cars Models n Europe



Battery Pipeline



Add labels for CATMAT, SOLBAT, NEXTRODE

Royce inst?

Value is added along manufacturing process

THE FARADAY INSTITUTION

Battery industry structure






Raw materials	Precursors	Electrodes + components	Cells	Modules + packs	Vehicle applications	2nd life + recycling
Lithium, nickel, cobalt, manganese, copper, aluminium, graphite Supply chain, price volatility Purity Ethics	Lithium carbonate vs hydroxide Cobalt, nickel and manganese sulphates Processing, single crystal vs polycrystalline	Active material, conductive additives, binders Mixing, coating, drying, calendaring Separators, current collectors, electrolytes	Cylindrical, pouch, prismatic Size, capacity Electrolyte filling Formation Lifetime Consistency	Pack design Thermal management system Battery management system Lifetime	Load profile Environmental conditions Servicing Residual value Real world performance	Residual capacity Safety Logistics Residual value Policy Economics

Key considerations

Chemicals

Industrial chemists

Mining and refining

Material suppliers

Cell suppliers

Tier 1

Low volume OEM

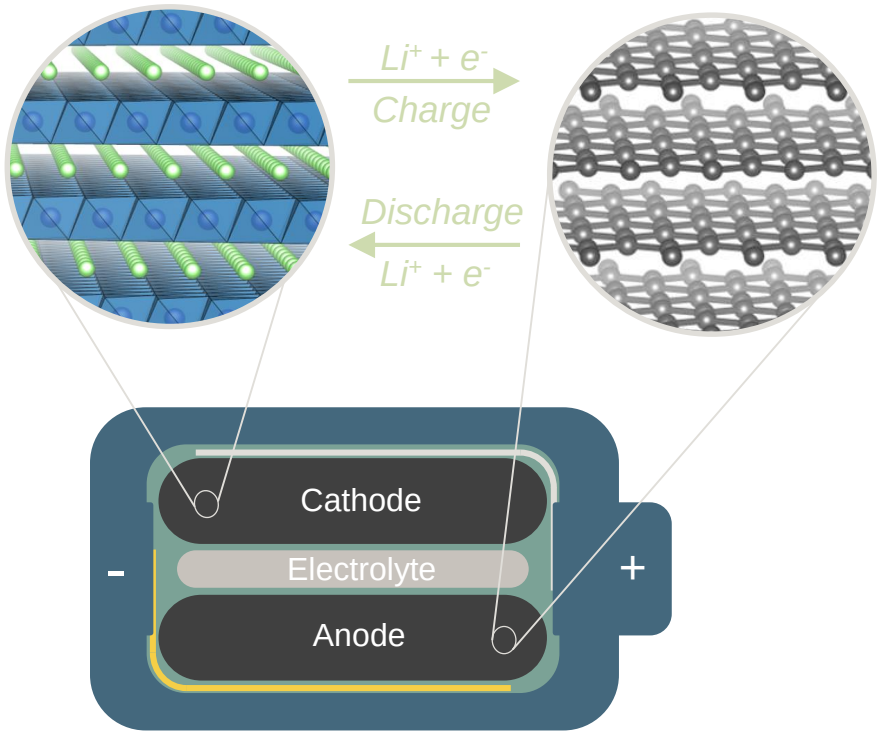
2nd user

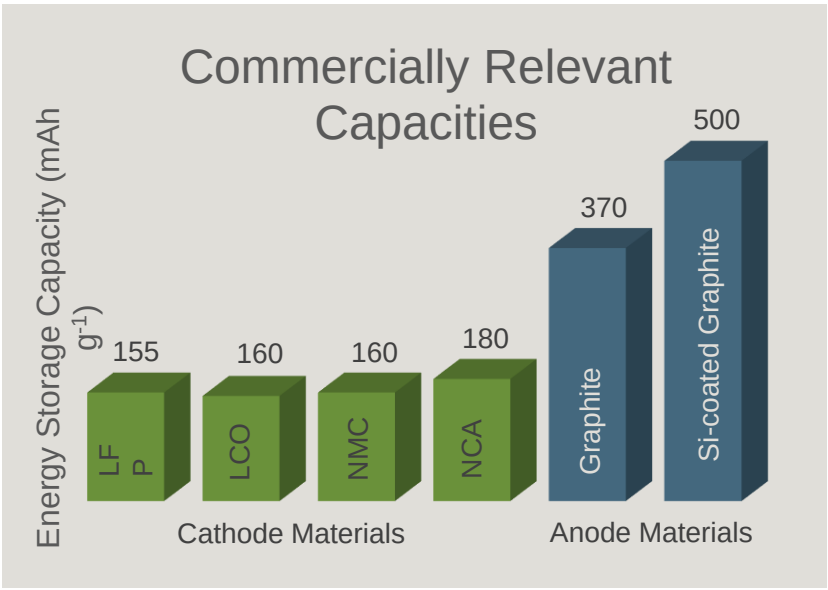
High volume OEM

Recycler

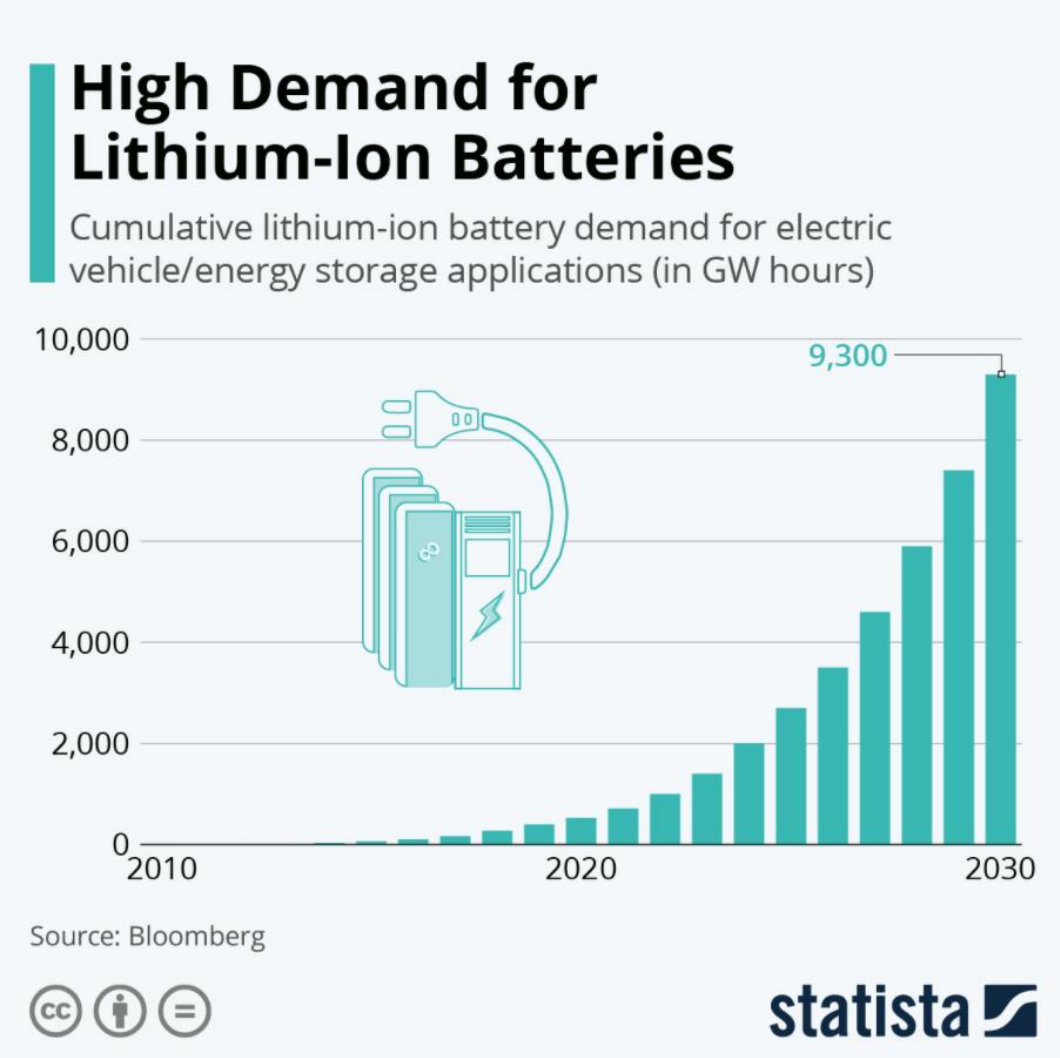
Adapted from content from Professor Dave Greenwood at Warwick Manufacturing Group
https://unsplash.com/photos/F_EooJ3-uTs

Fundamentals of a Li-ion Battery





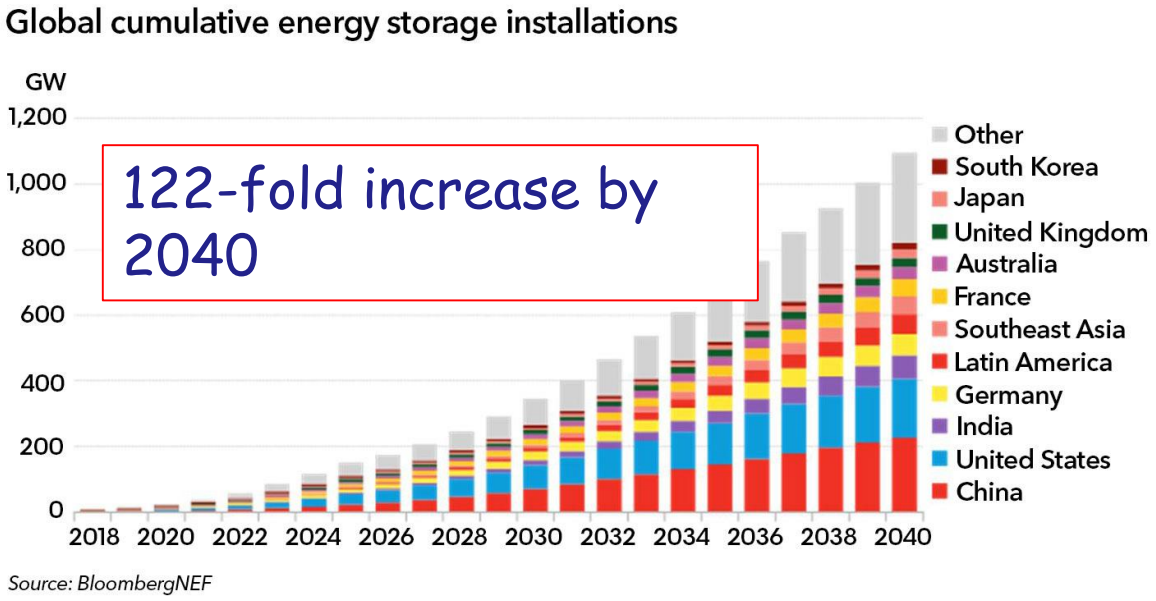
Growth in Lithium Batteries



Exponential Growth in Storage

Major drivers for growth:

- Energy shifting
- Peak demand
- Lower bills for consumers

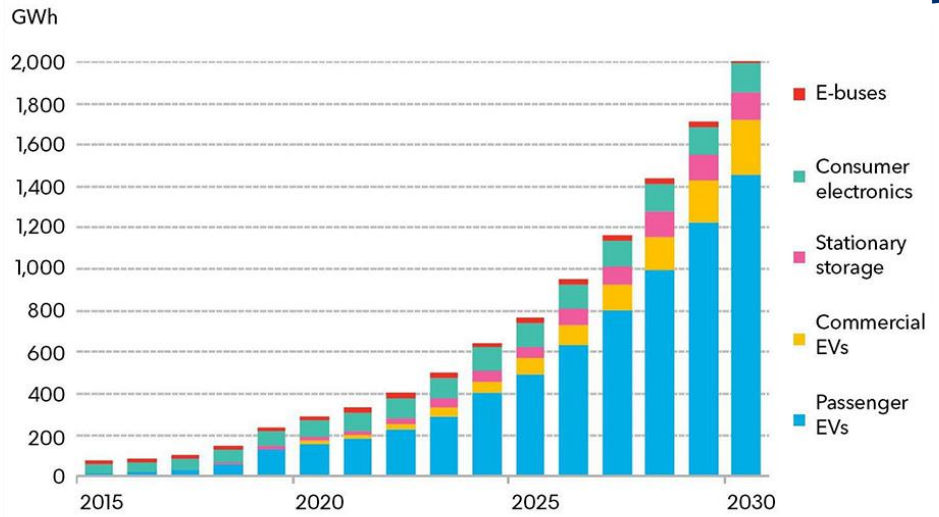


Intermittent renewables set to account for 40% of the world's electricity by 2040

Growth in utility-scale installations

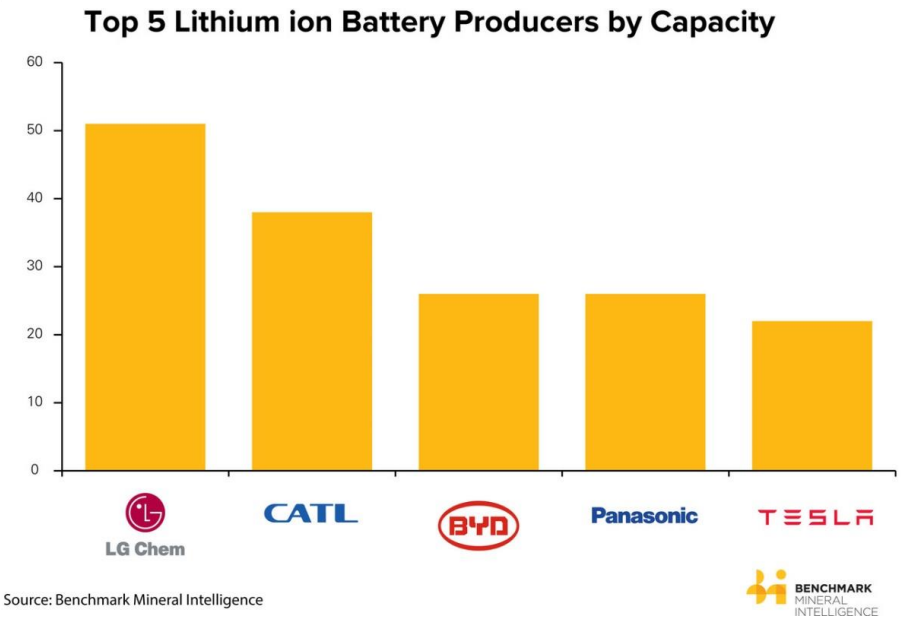
$662 billion of investment

Global Li-ion Battery Market



Source: BloomberaNEF. Avicenne

- Rapid market growth predicted
- Driven by the transition from ICE to EV



Source: Benchmark Mineral Intelligence

- Market dominated by Korean, Chinese and Japanese manufacturers

Lithium-ion Batteries Cost (Cell Level)

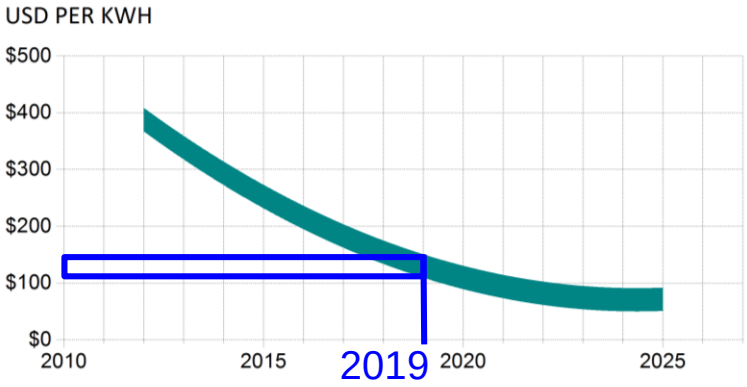
Increasing manufacturing capacity

Chinese state support (as for solar)

Technological advances

Decrease

$ COST $



$

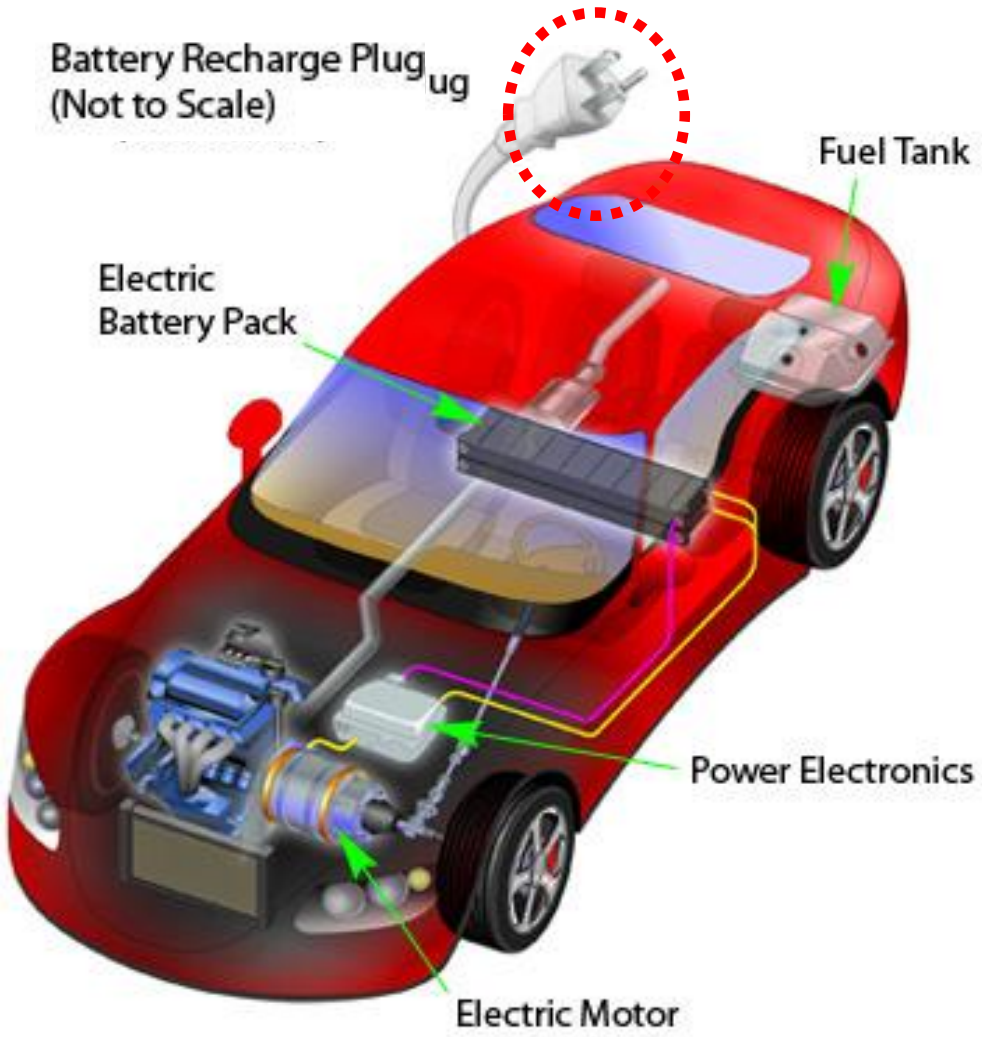
Increase

$ COST $

Cost of raw materials

Can supply grow fast enough to keep up with demand?

Green Light for Electric Cars



Batteries for EVs

Need advances in lithium batteries

Materials understanding & discovery

Device manufacturing & performance

Need New Cathode Materials

Cathode (oxide) vs Anode (graphite)