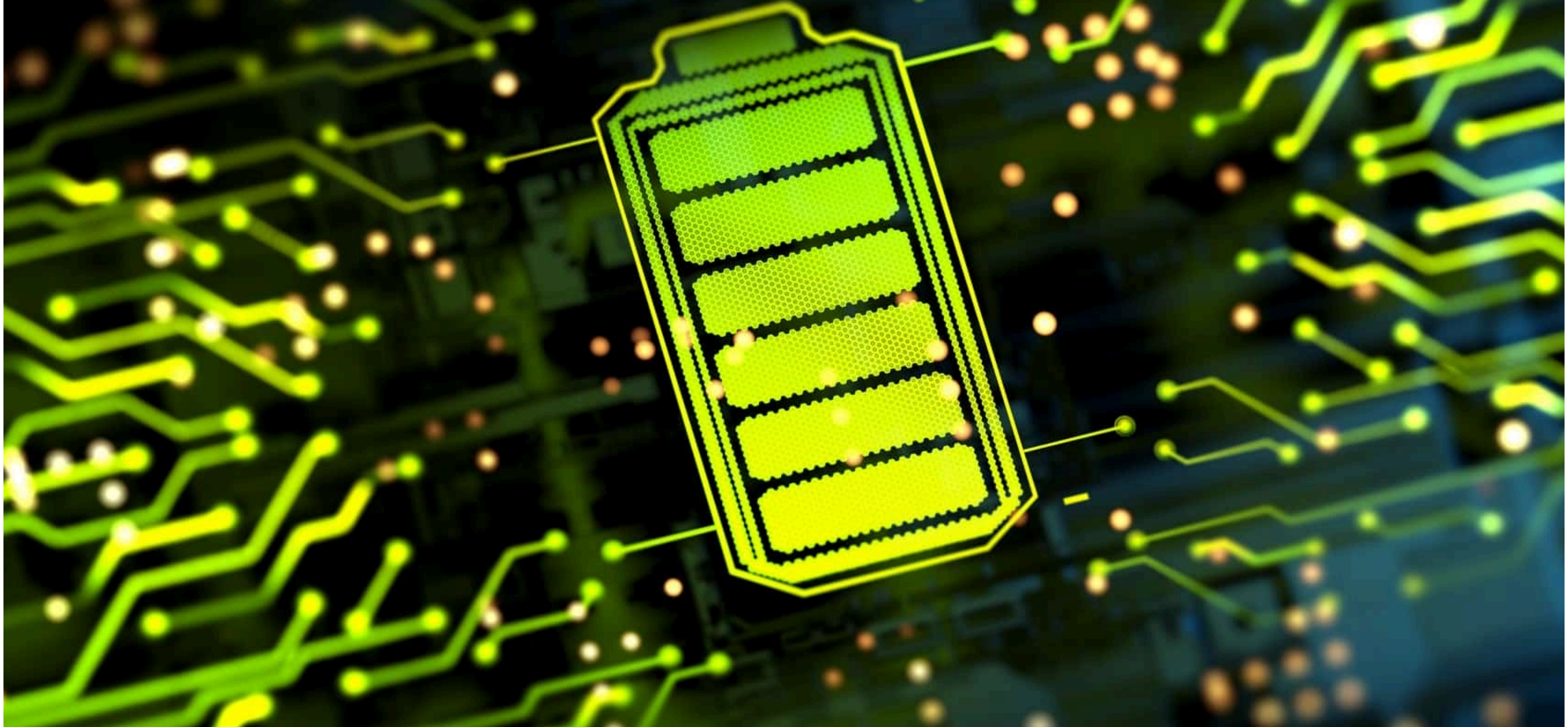
Batteries Part III: From Li-ion to grid-scale storage and autonomous materials discovery

BATTERY 2030+

47202: Introduction to Future Energy; 2023-11-14



Prof. Tejs Vegge, teve@dtu.dk, DTU Energy

Technical University of Denmark

Increasing the Energy and Power Density

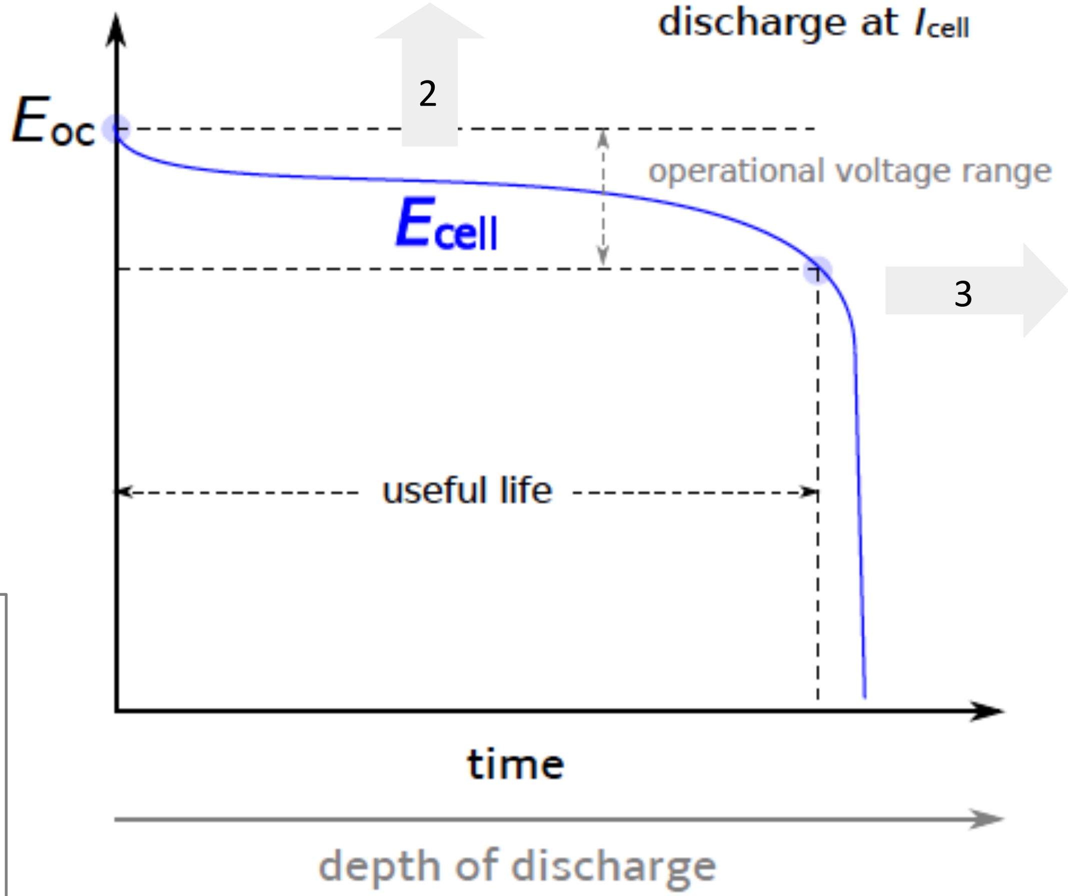
Three options for increasing the energy density:

1) use light(er) and dense(r) materials to increase gravimetric and volumetric energy density
2) increase cell voltage
3) increase capacity (amount of Li+ stored per weight / volume)

$$\text{energy} = \overline{E}_{\text{cell}} \cdot \underbrace{I_{\text{cell}} \cdot t}_{\text{capacity} \quad Q\text{ (charge)}}$$

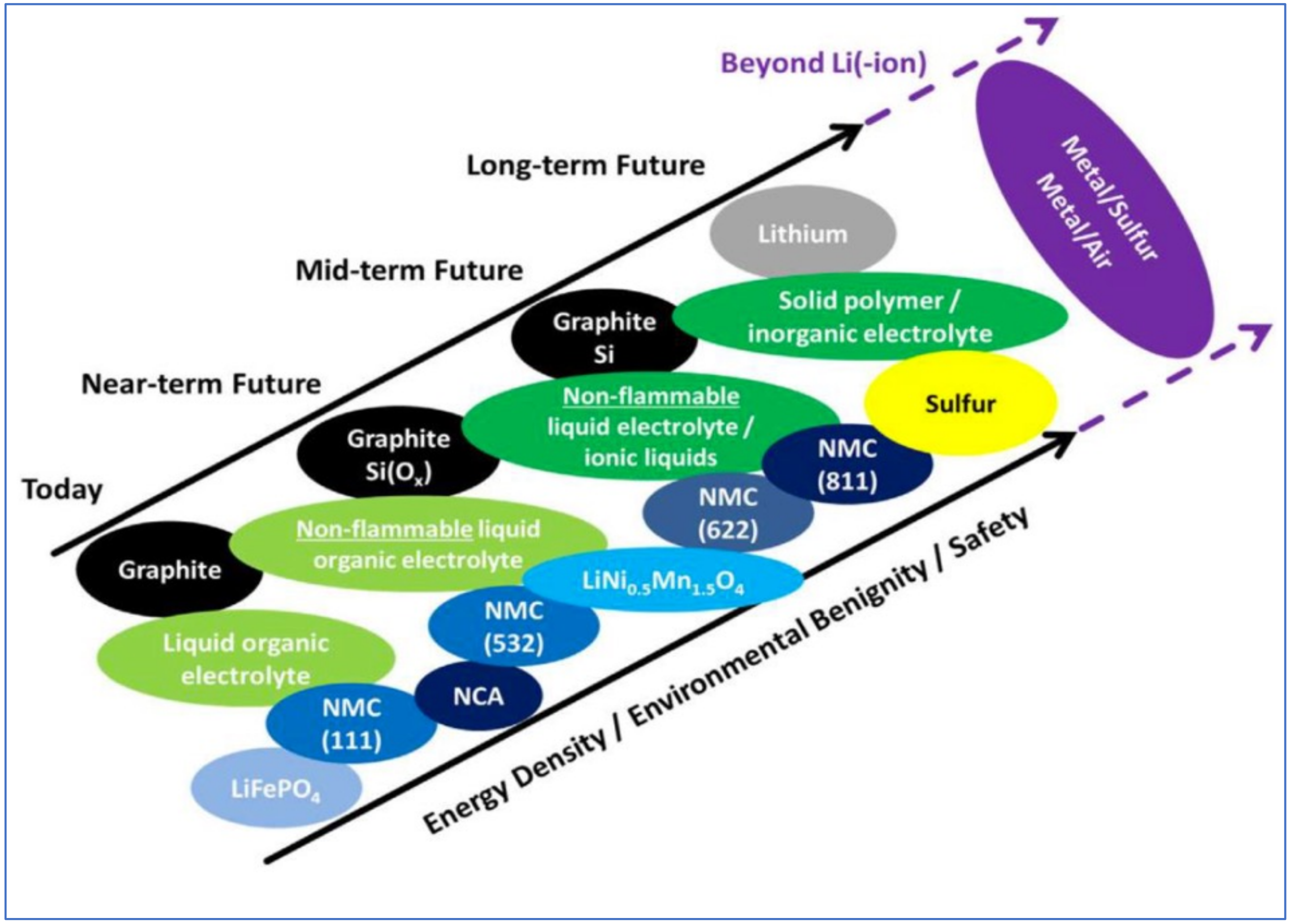
$$\text{power} = I \cdot E$$

A discharge curve:



Next generation battery materials

- How do we get better batteries?
- …and how do we get them faster

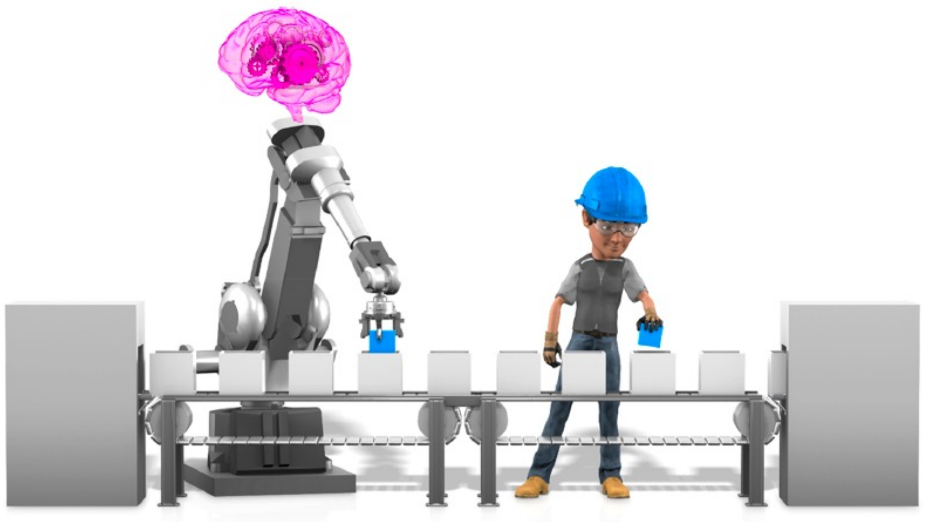


Edström, Dominko, Fichtner, Otuzewski, Perraud, Punckt, Tarascon, Vegge, Winter, BATTERY 2030+ Roadmap (2020)

Can computer simulations and AI help us get better batteries faster?

A multi-pronged AI-accelerated approach

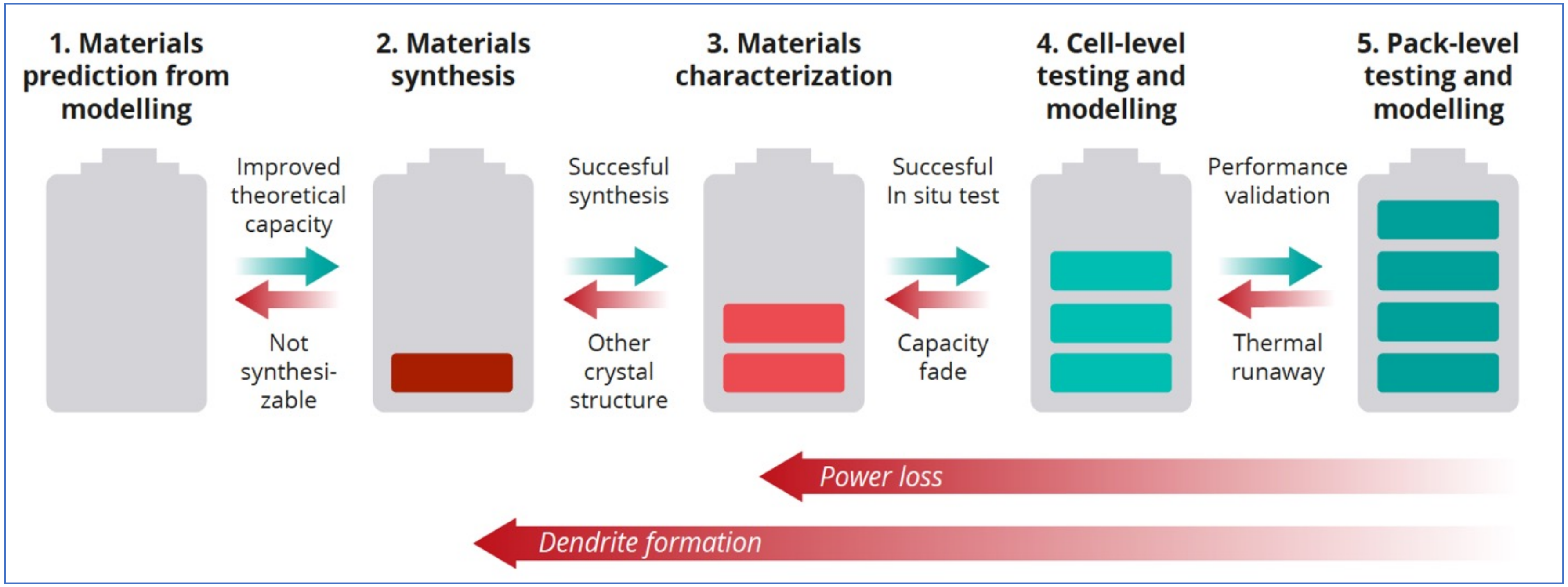
- Inverse design and computational materials discovery
- Getting more out of existing batteries
- Develop autonomous materials discovery platforms



Lombardo, Vegge, Johansson, Franco, et al. Chem. Rev. 10.1021/acs.chemrev.1c00108 (2021)

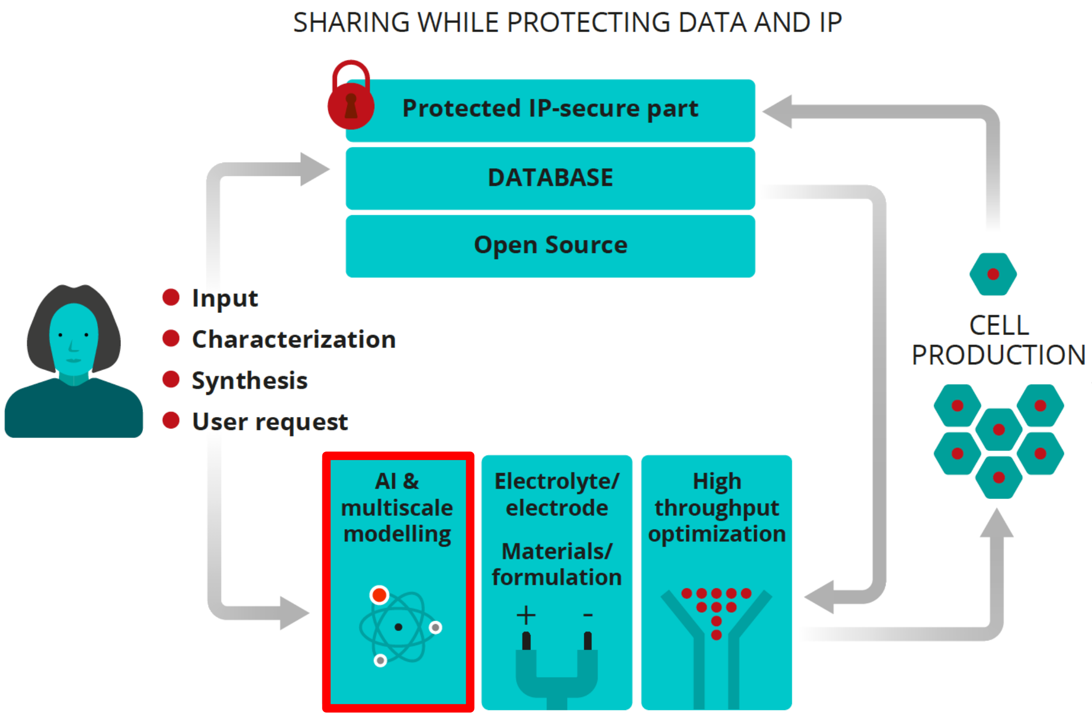
Current Battery Development is Sequential

- Li-ion: a 20-years discovery & development process
- Can AI, simulations and closed-loop discovery accelerate the discovery & development process?



An AI-accelerated closed-loop battery discovery infrastructure

Accelerated closed-loop discovery using AI-accelerated models & procedures



Vegge, Tarascon, Edström, Adv. Energy Mater. 11, 2100362 (2021); Fisker-Bødker, Moretti, Chang, Kiebach, Vegge (2022)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement #957189

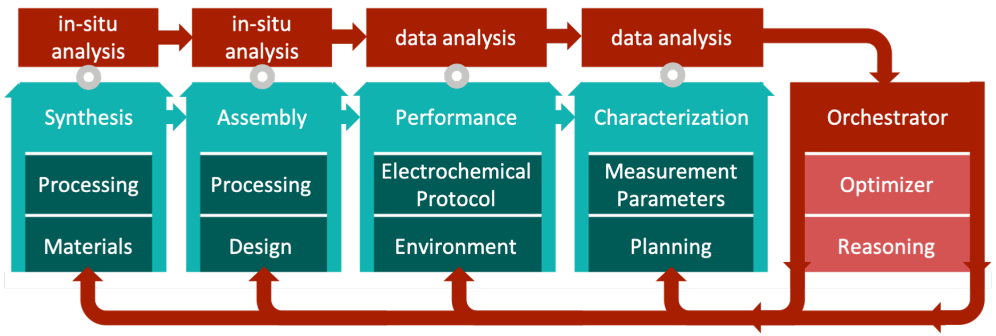
BIG-MAP: Battery Interface Genome – Materials Acceleration Platform

Reinventing the way we invent batteries

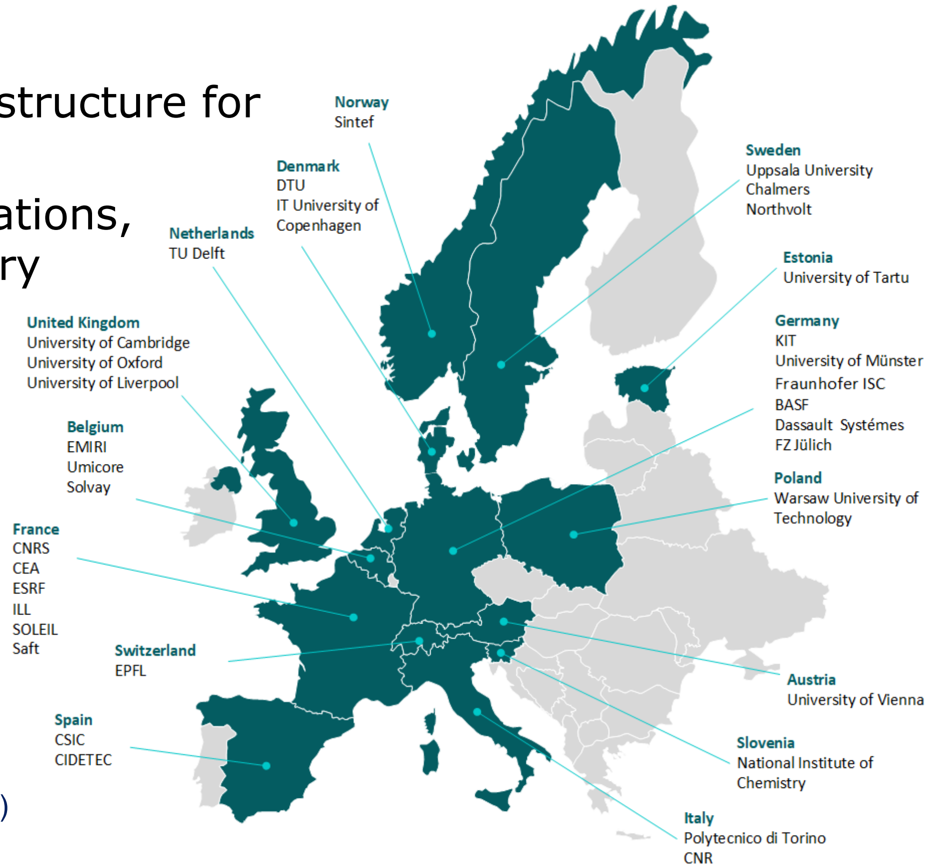
Developing an AI-accelerated digitalized infrastructure for the European Battery Community

34 partners from academia, research organizations, large-scale research infrastructure and industry

Watch video on www.big-map.eu



Vegge et al., Adv. Energy Mater, DOI: 10.1002/aenm.202102698 (2021)



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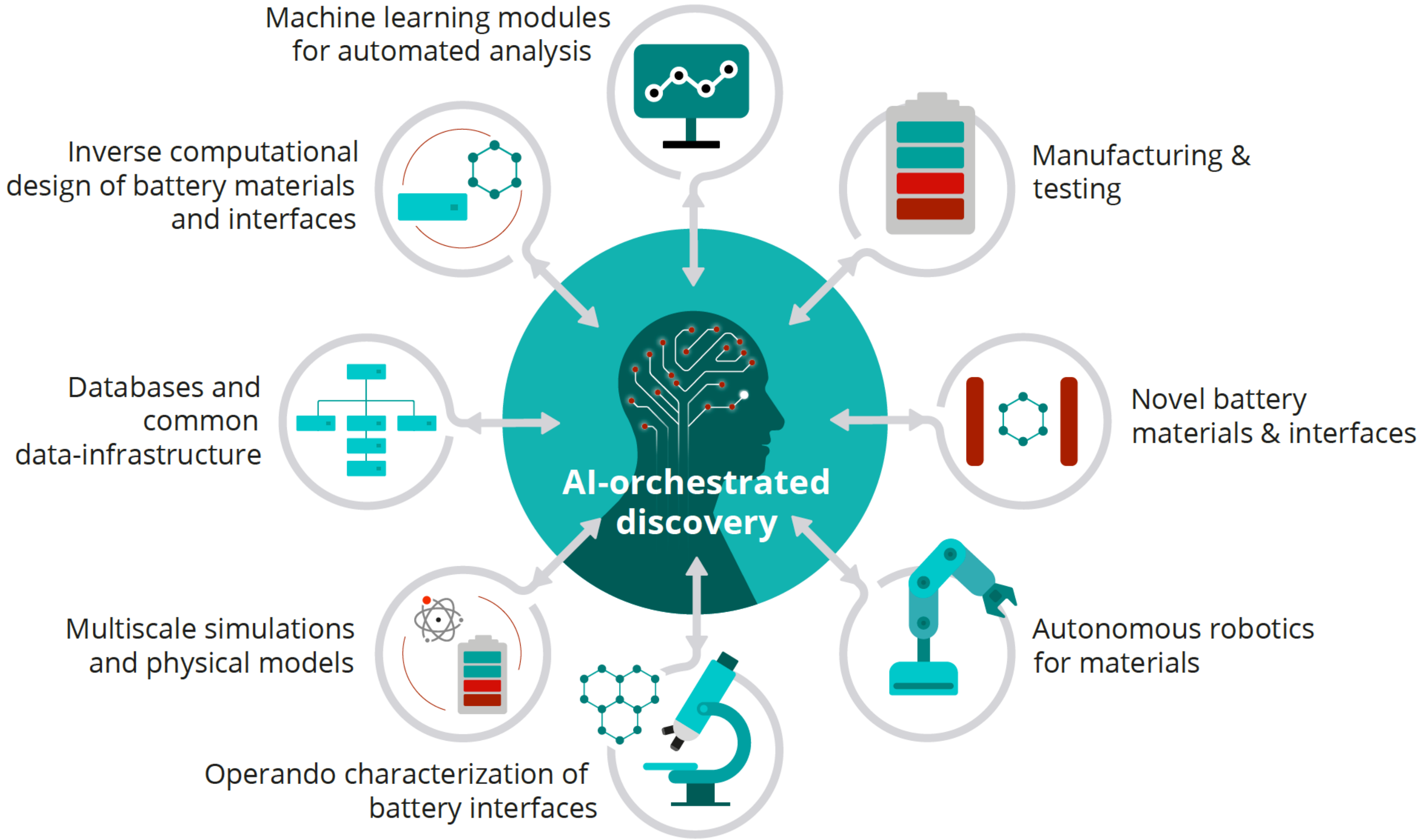
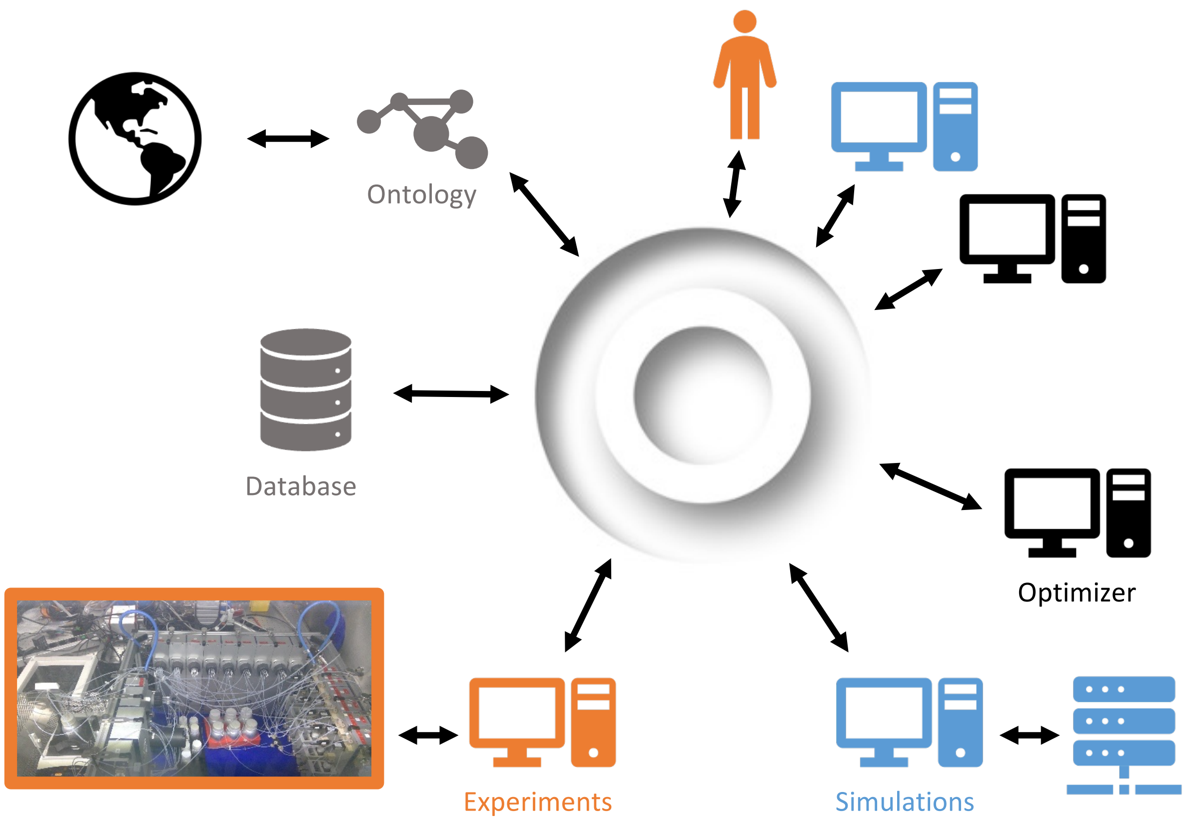
DTU Energy, Technical University of Denmark

Accelerating battery discovery and development



DTU Energy, Technical University of Denmark

FINALES: Fast INtention-Agnostic Learning Server



- broker server
- asynchronous
- append only
- data structures (ontology linked)
- hardware independent (request results, not procedures)
- multitenancy

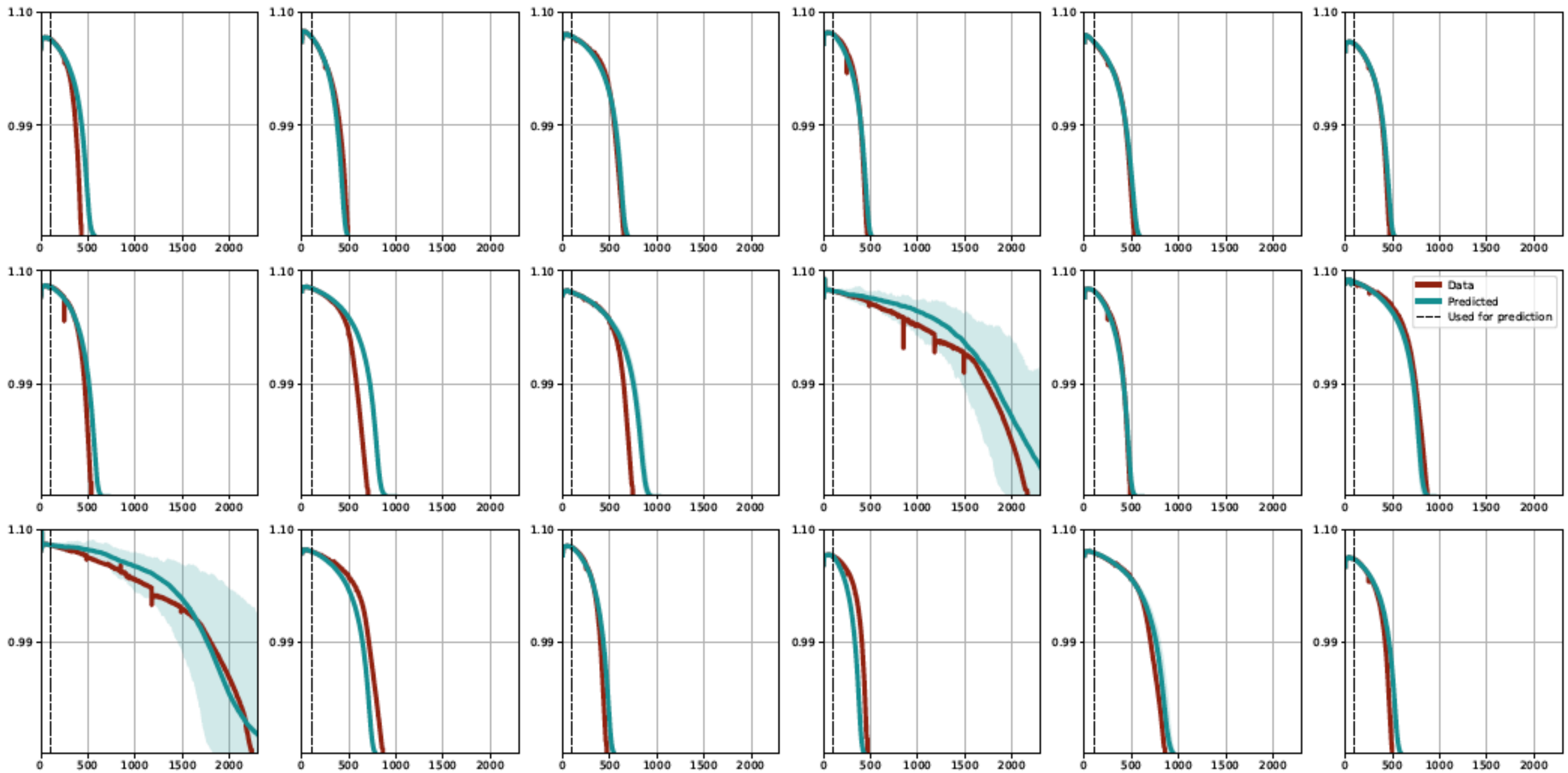
Vogler, et al., Matter, 10.26434/chemrxiv-2022-grgrd (2022)

DTU Energy, Technical University of Denmark

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

AI-guided Uncertainty-aware prediction of Battery EOL

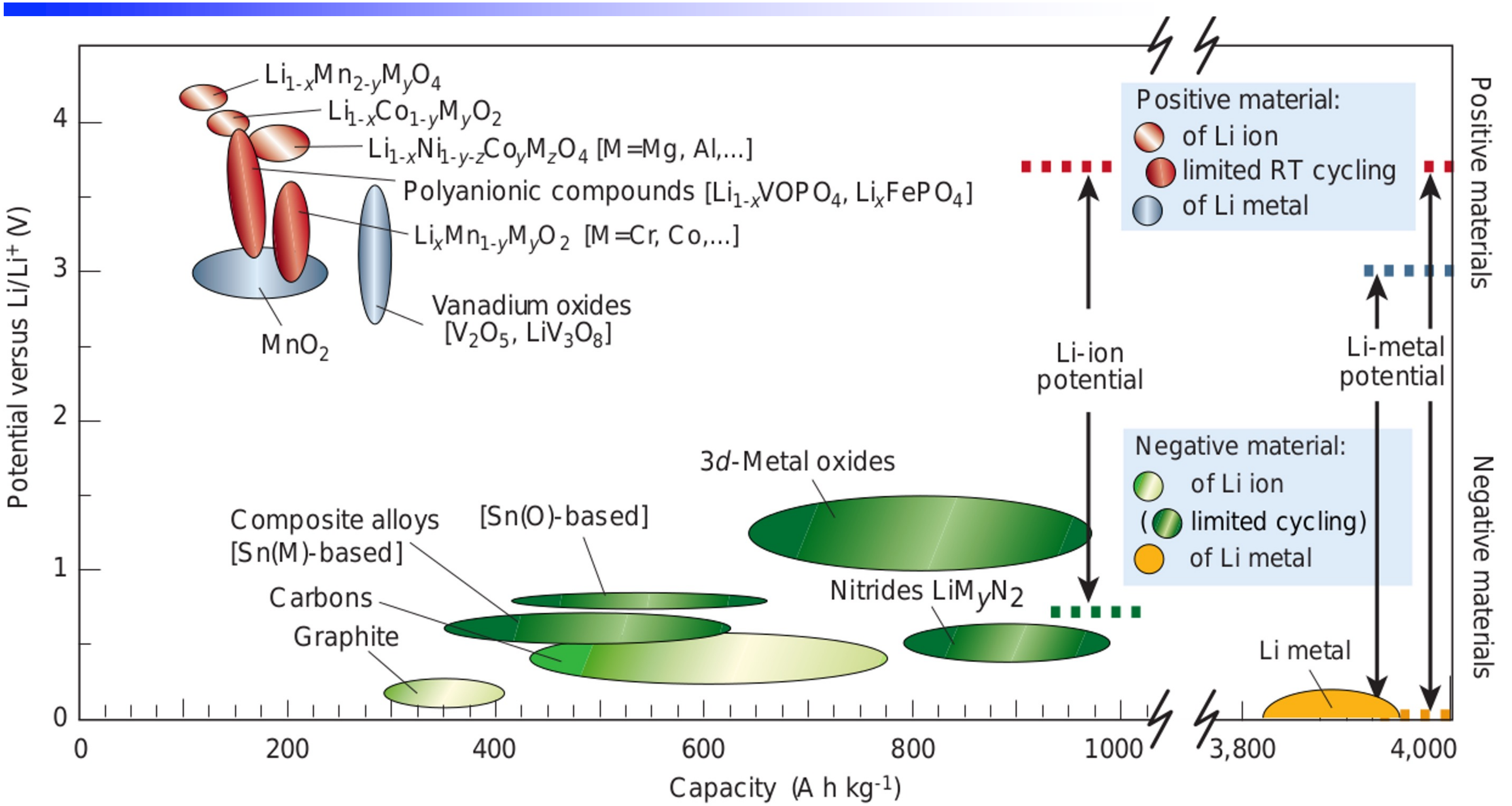
- Calibrating uncertainty with graph-based neural network ensembles
- Deep learning for faster predictions of battery End Of Life with uncertainty estimates



Busk, Jørgensen, Bhowmik, Schmidt, Winther, Vegge, Machine Learning: Science and Technology 3, 015012 (2022)
Rieger, Flores, Nielsen, Norby, Ayerbe, Winther, Vegge, Bhowmik, Digital Discovery 2, 112-122 (2023)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement #957189

Li-ion Battery Materials – Potential vs Capacity



A moderate increase in voltage possible, e.g. $Li_xNi_{0.5}Mn_{1.5}O_4$ operates at ~4.7 V

→ no dramatic increase in capacity (C_T = 147 mAh/g), but energy density increases!

Source: Tarascon, J.-M.; Armand, M. Issues and Challenges Facing Rechargeable Lithium Batteries. Nature 2001, 414 (6861), 359–367 DOI: 10.1038/35104644.

High Voltage Cathodes for Li-ion Batteries

- Higher voltages (>4.5 V vs. Li/Li^+) and higher capacities
- Cathodes like Li_2MnO_3–$LiNi_{0.5}Mn_{0.5}O_2$, $LiMn_{1.5}Ni_{0.5}O_4$, $LiCoPO_4$, and $LiNiPO_4$, have operating voltages between 4.7 and 5.2 V
- Key limitation: electrolytes with very high electrochemical stability

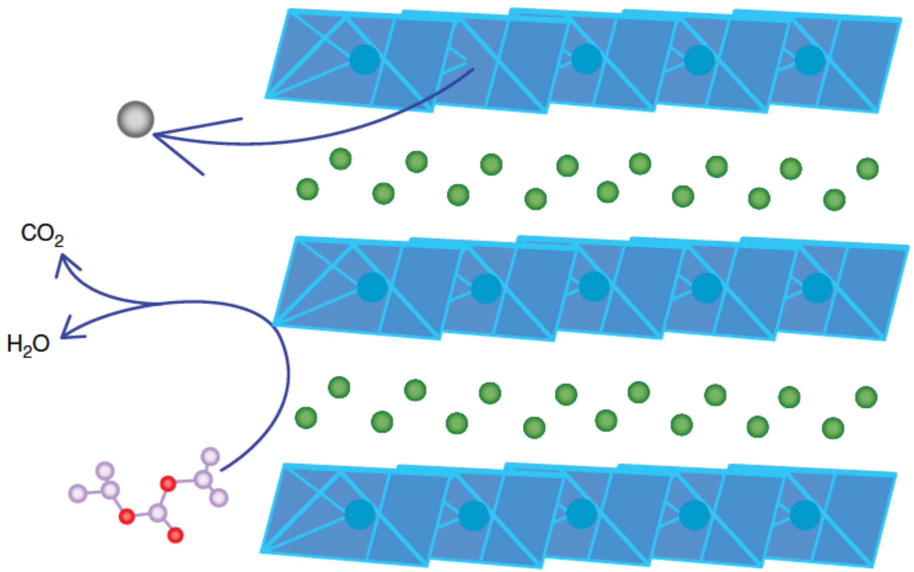
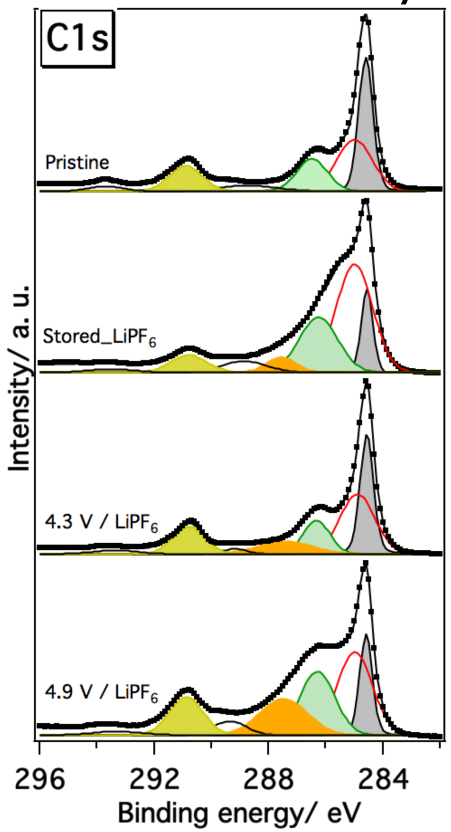


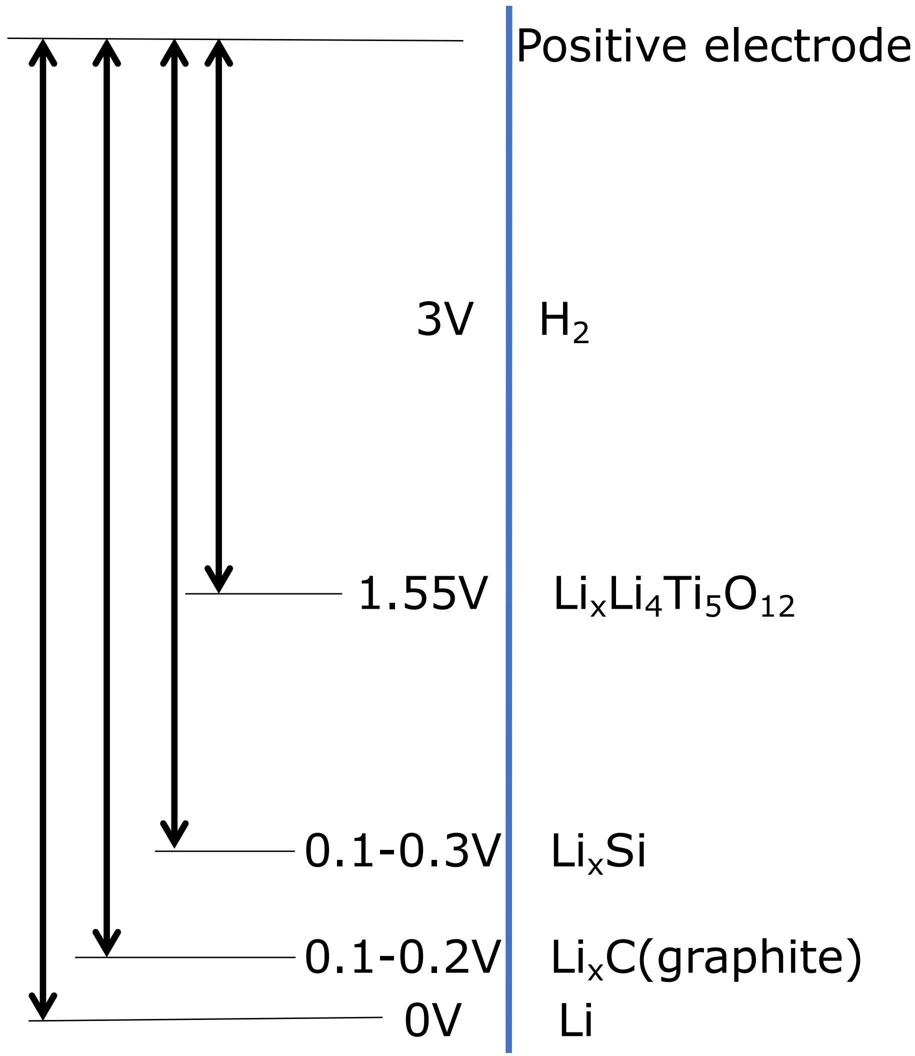
FIGURE 4 Dissolution of metal elements and decomposition of electrolyte at a high-voltage cathode surface.



Younesi, Christiansen, Loftager, Garcia-Lastra, Vegge, Norby, Holtappels, Chem. Sus. Chem. 8, 3213 (2015)
Scrosati, Abraham, Schalkwijk, Hassoun, Lithium Batteries: Advanced Technologies and Applications, Wiley (2013)

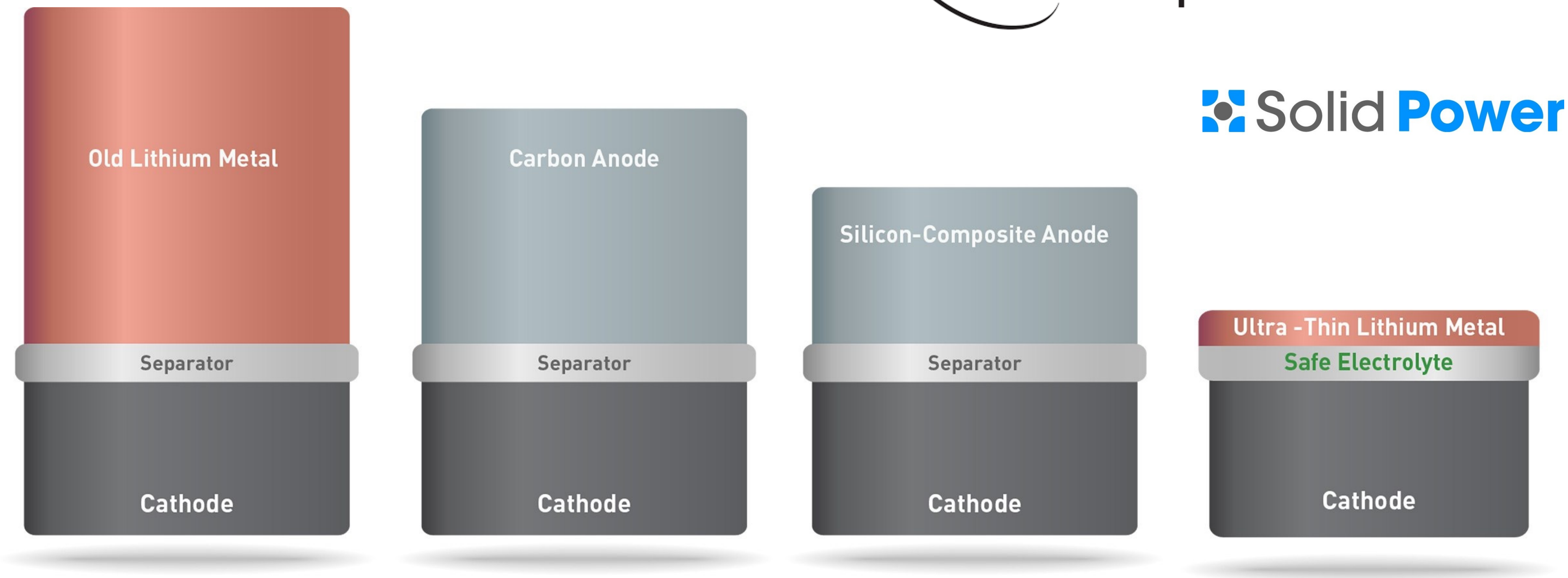
High Capacity Anodes for Lithium Batteries

- Li-metal anodes are unsafe, so graphite is used (Li_xC_6:372 mAh/g)
- Si, Sn, Al, Bi can alloy with Li ($SiLi_4$ @ 4200 mAh/g), but undergoes a ~400% change in volume
- Significant interest for such anodes in the automotive industry



Hassan, Batmaz, Li, Wang, Xiao, Yu, Chen, Nature Communication 6, 8597 (2015)

Solid state batteries

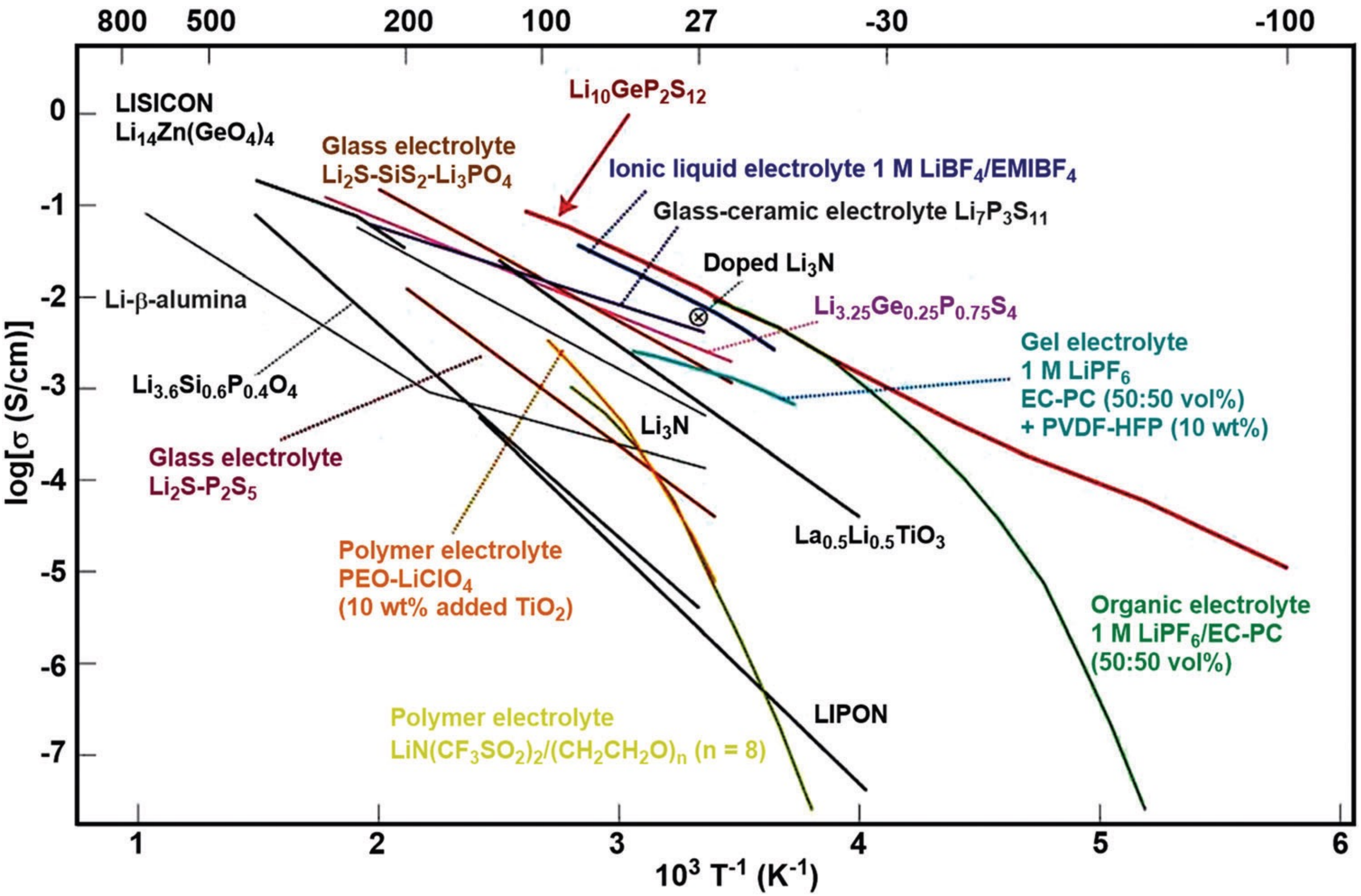


Gen 0	**Gen 1**	**Gen 2**	**Gen 3**
Li-Metal	**Li-ion**	**Li-ion**	**Li-Metal**
100-200 Wh/kg	200-250 Wh/kg	250-300 Wh/kg	400-500 Wh/kg
200-300 Wh/L	600 Wh/L	700 Wh/L	1200 Wh/L
Dangerous	Safe	Safe	Safest

IRENA, Electricity Storage and Renewables: Costs and Markets to 2030 (2017)

Conductivity of solid Li-ion electrolytes

- The Li-ion conductivity remains (too) low



Lin et al, Chem. Soc. Rev. 45, 5848-5887 (2016)

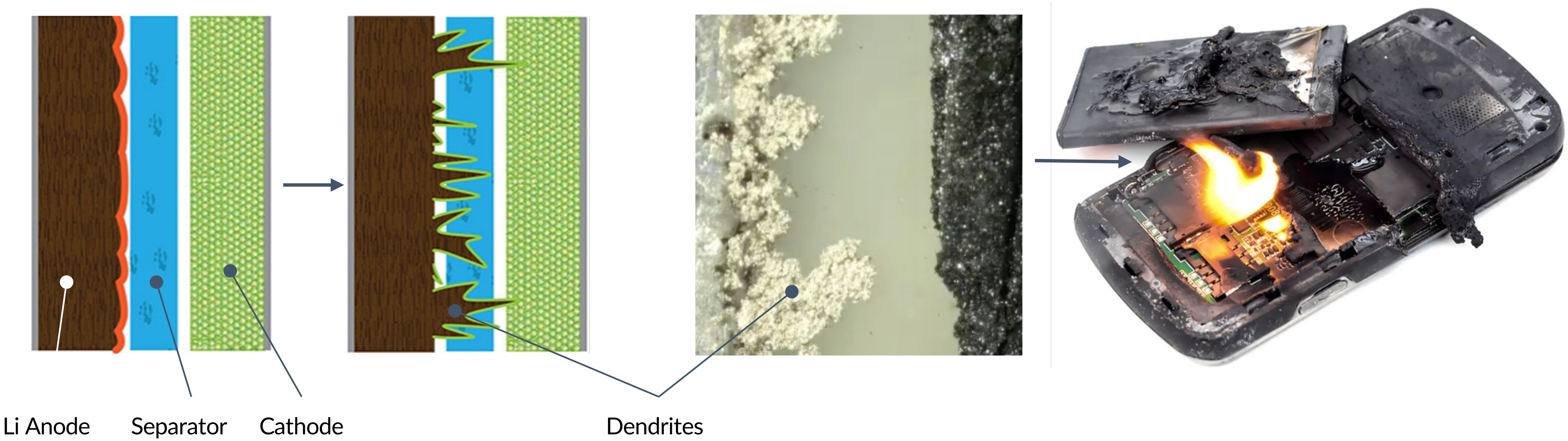
Are all-solid-state batteries there yet?

- Almost…
- Toyota expect to mass-produce solid-state batteries by 2027 or 2028
- Claim: A range of 1,200km and a charging time of 10 minutes or less

Toyota (2023)

Dendrite growth in Li(s) batteries

Dendrite growth plagues the development of future all-solid-state and Li-metal batteries

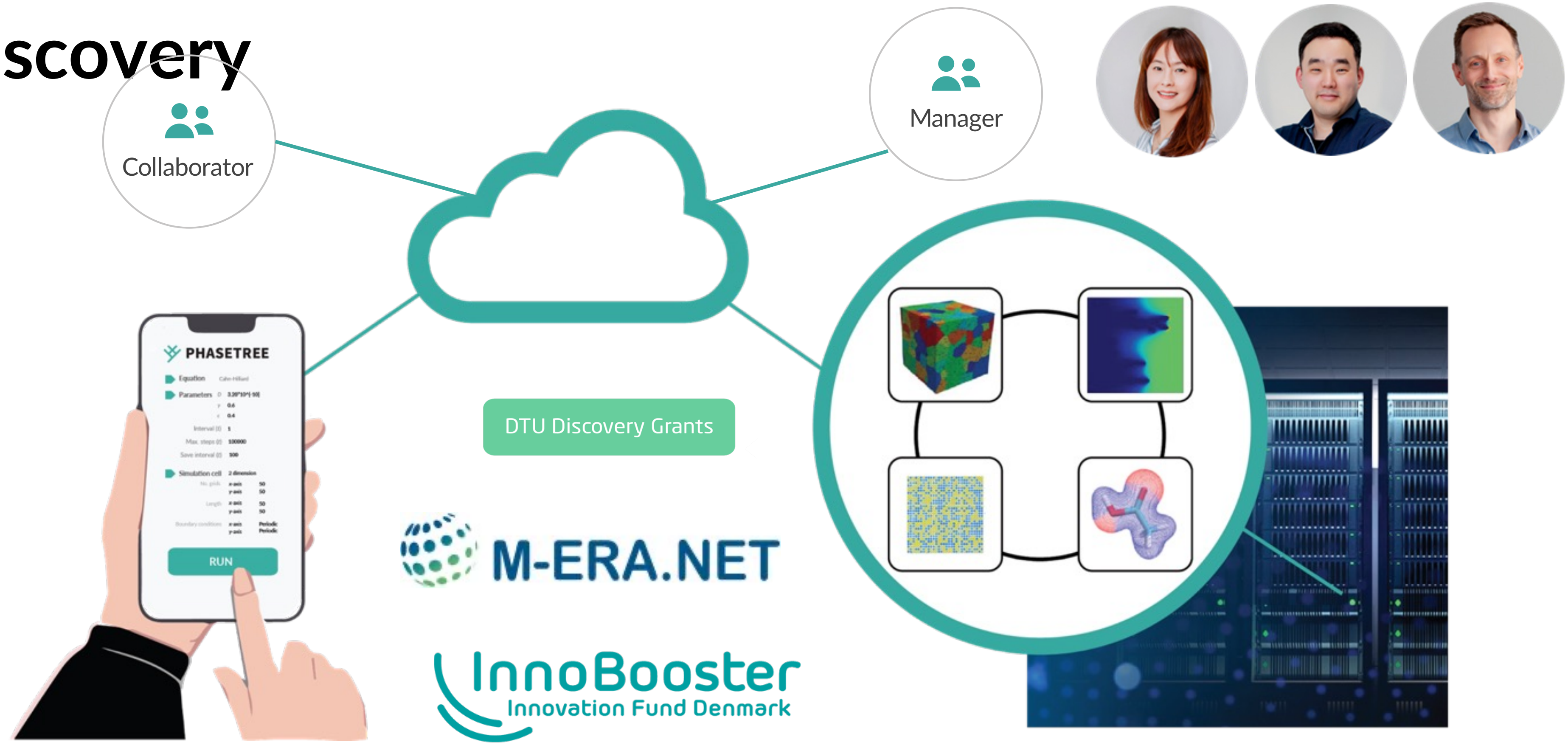


Performing atomic-scale-informed phase field simulations of dendritic growth

Jeon, Gil Ho, Vegge, Chang, ACS Appl. Mater. Inter 14, 15275–15286 (2022)

PHASETREE

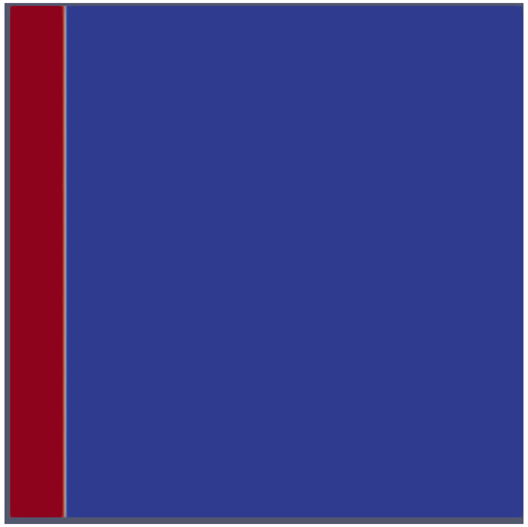
Virtual Platform for Accelerated Materials Discovery



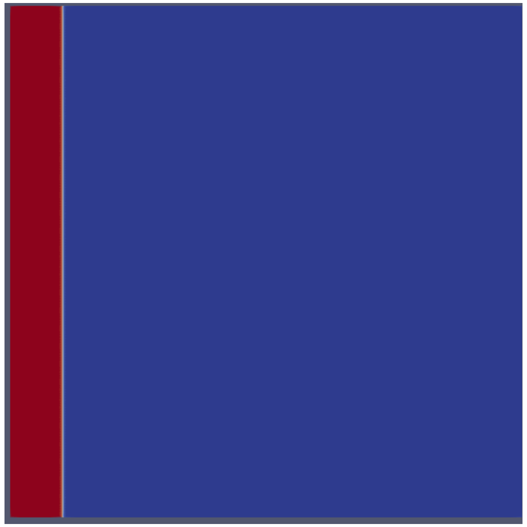
Dendrite growth in Li(s) batteries

- Dendrite growth is a leading cause of failure in Li-metal batteries
- Modifying materials composition or use conditions to suppres dendrite growth

V = -0.3 V



V = -0.45 V



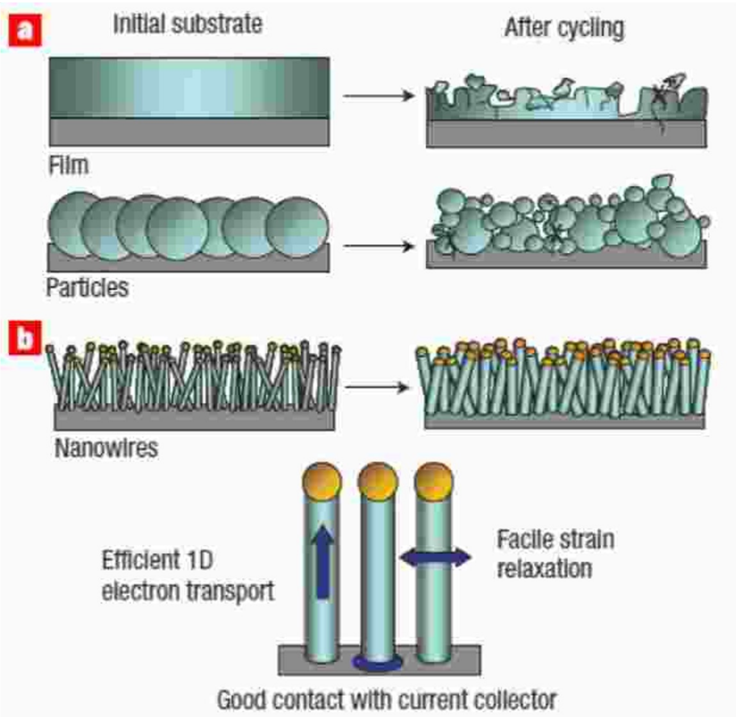
Jeon, Gil Ho, Vegge, Chang, ACS Appl. Mater. Inter 14, 15275–15286 (2022)

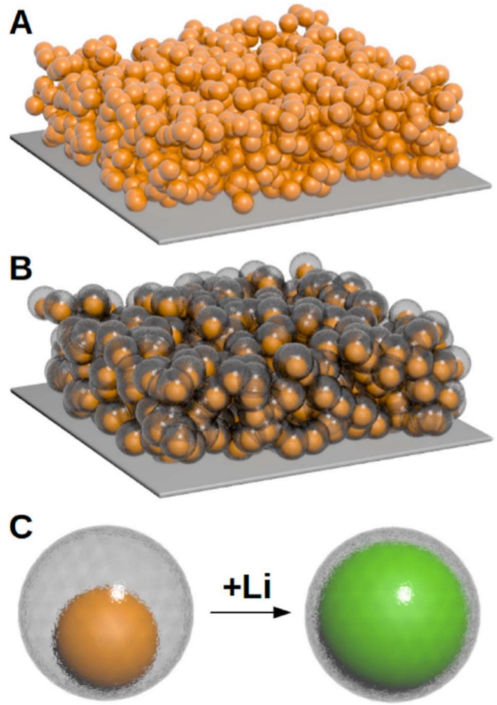
Si-anodes

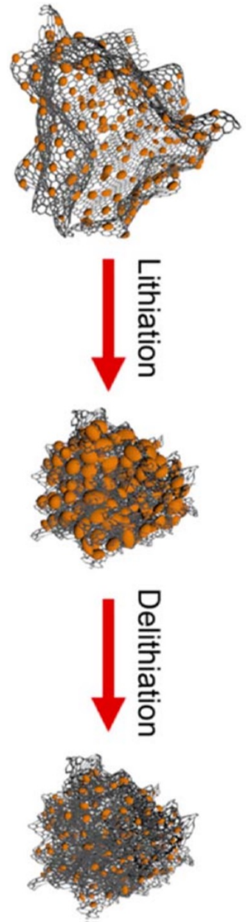
- Silicon can alloy with Lithium resulting in compositions up to **$Li_{4.4}Si$** yielding
- Theoretical capacity of **4200 mAh/g**

→ more than 10x the capacity of graphite (372 mAh/g)!

- Operates at ~ **0.4 V**
- But: alloying is accompanied by up to a 300% volume expansion...





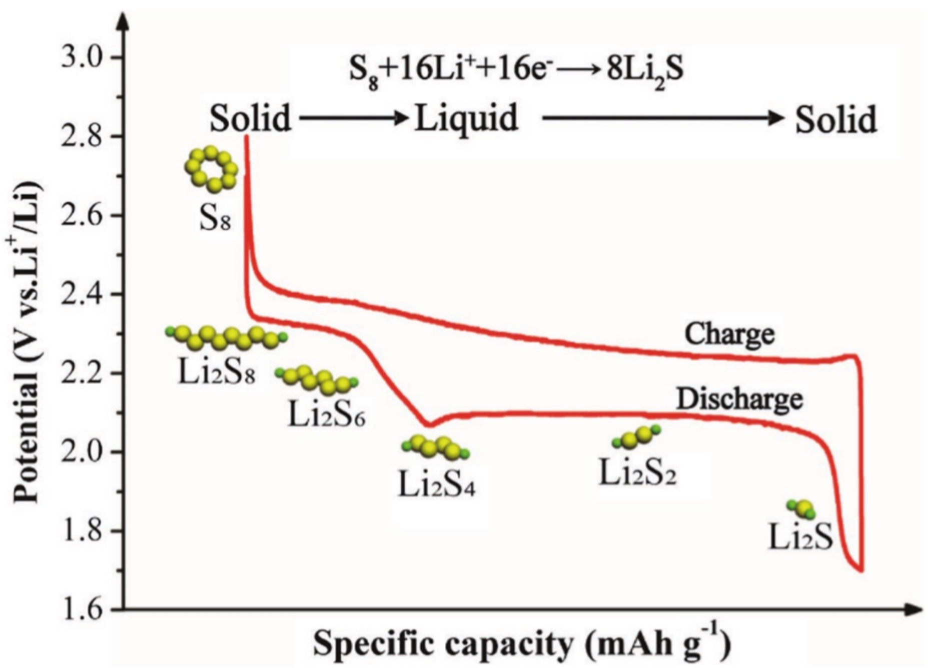


A lot of research dedicated to ways of managing the volume expansion problem

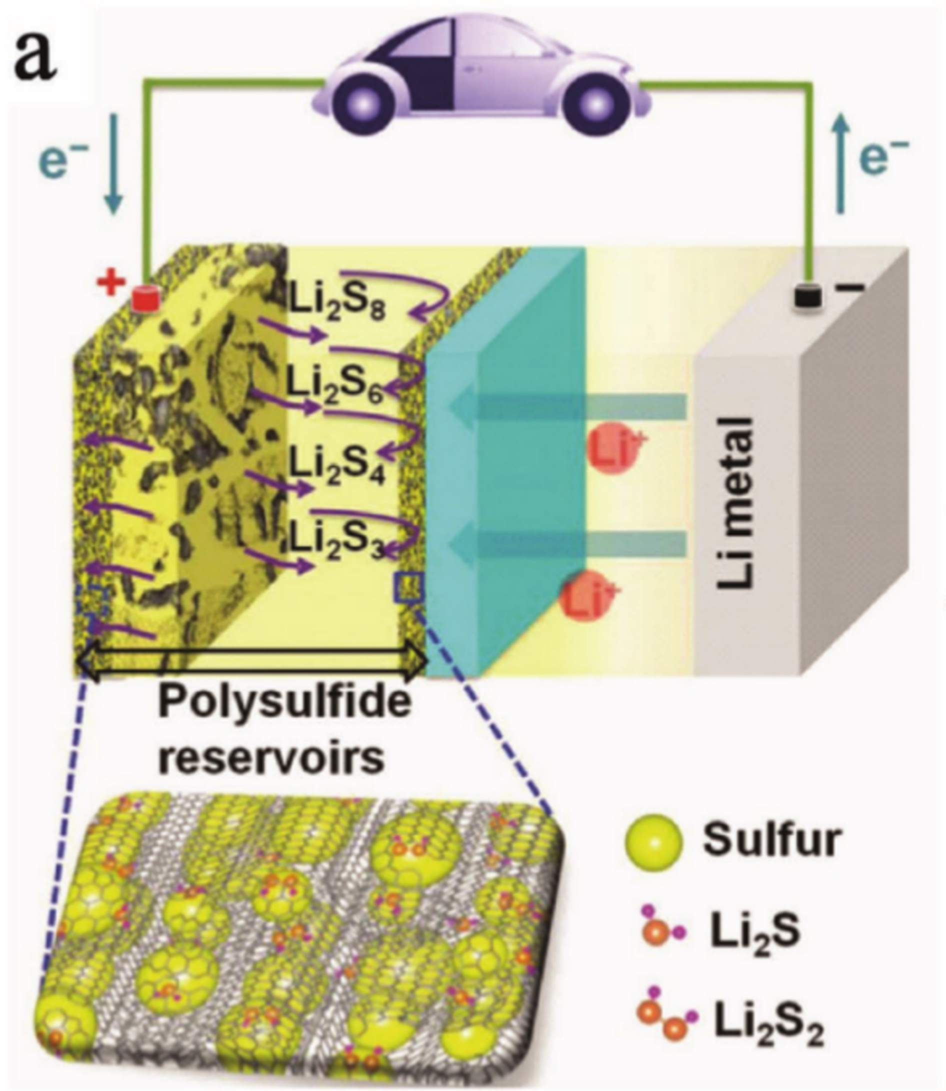
(→ reduced attainable capacity)

Zuo, X.; Zhu, J.; Müller-Buschbaum, P.; Cheng, Y.-J.
Silicon Based Lithium-Ion Battery Anodes:
A Chronicle Perspective Review. Nano Energy 2017, 31, 113–143
DOI: 10.1016/j.nanoen.2016.11.013.

Low Temperature Metal-Sulfur Batteries



Utilizing low cost materials,
and has a high theoretical capacity,
but have issues with the so-called
poly-sulfide shuttle.
(transport of cathode material to anode
and vice versa...)



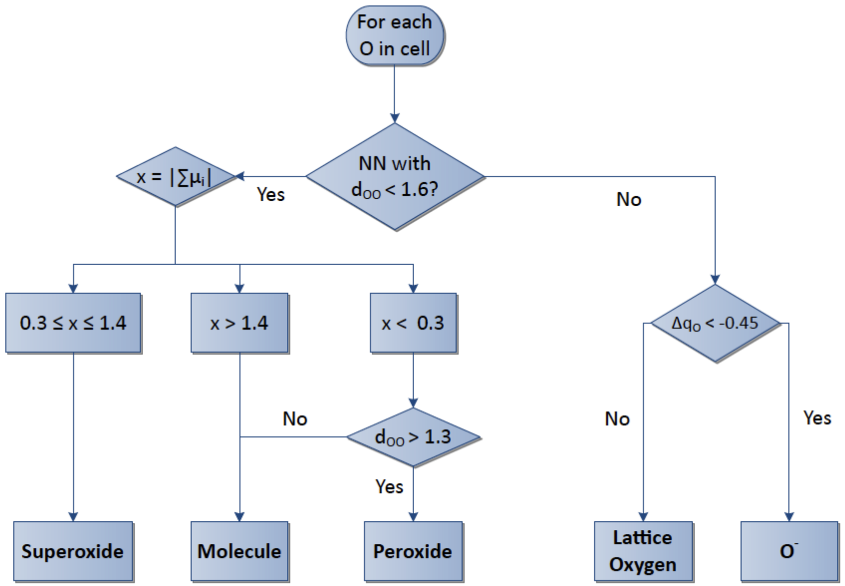
(1) Fang et al, More Reliable Lithium-Sulfur Batteries: Status, Solutions and Prospects. Advanced Materials 2017, 1606823 DOI: 10.1002/adma.201606823.
(2) Manthiram et al, Lithium-Sulfur Batteries: Progress and Prospects. Advanced Materials 2015, 27 (12), 1980–2006 DOI: 10.1002/adma.201405115.

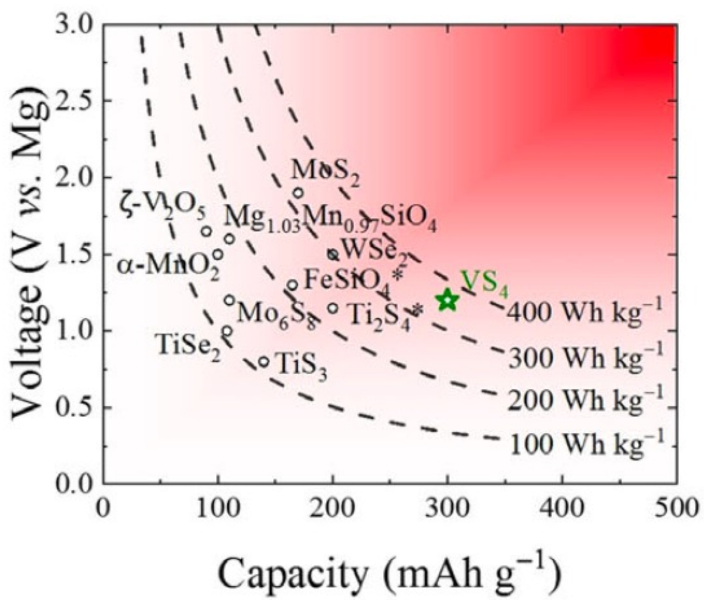
Utilizing anionic redox in battery electrodes

Automated procedures for detecting the unexpected, e.g., on-the-fly detection of anionic redox processes (could increase capacity dramatically)

Anionic redox in Li-rich (Li_xMnO_3, Li_xVO_2F)

and multi-valent (VS_4) Mg battery electrodes



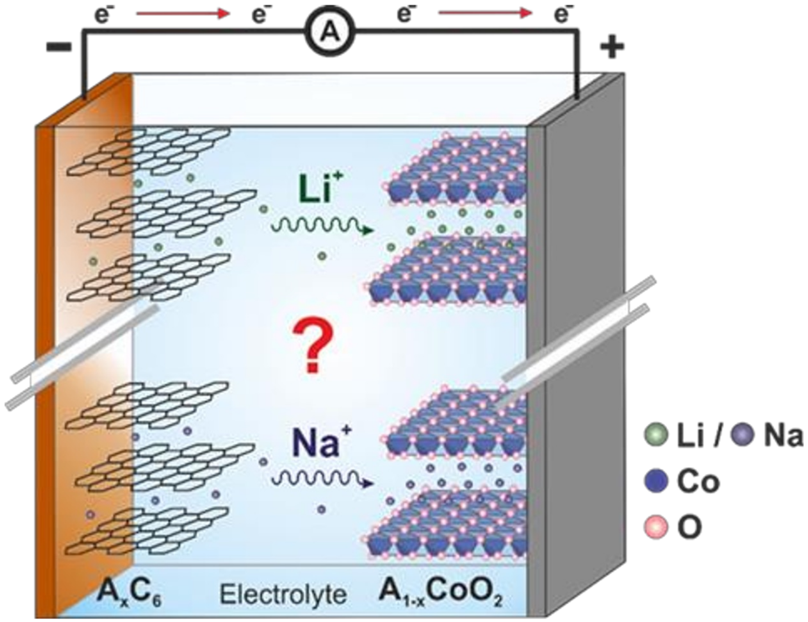


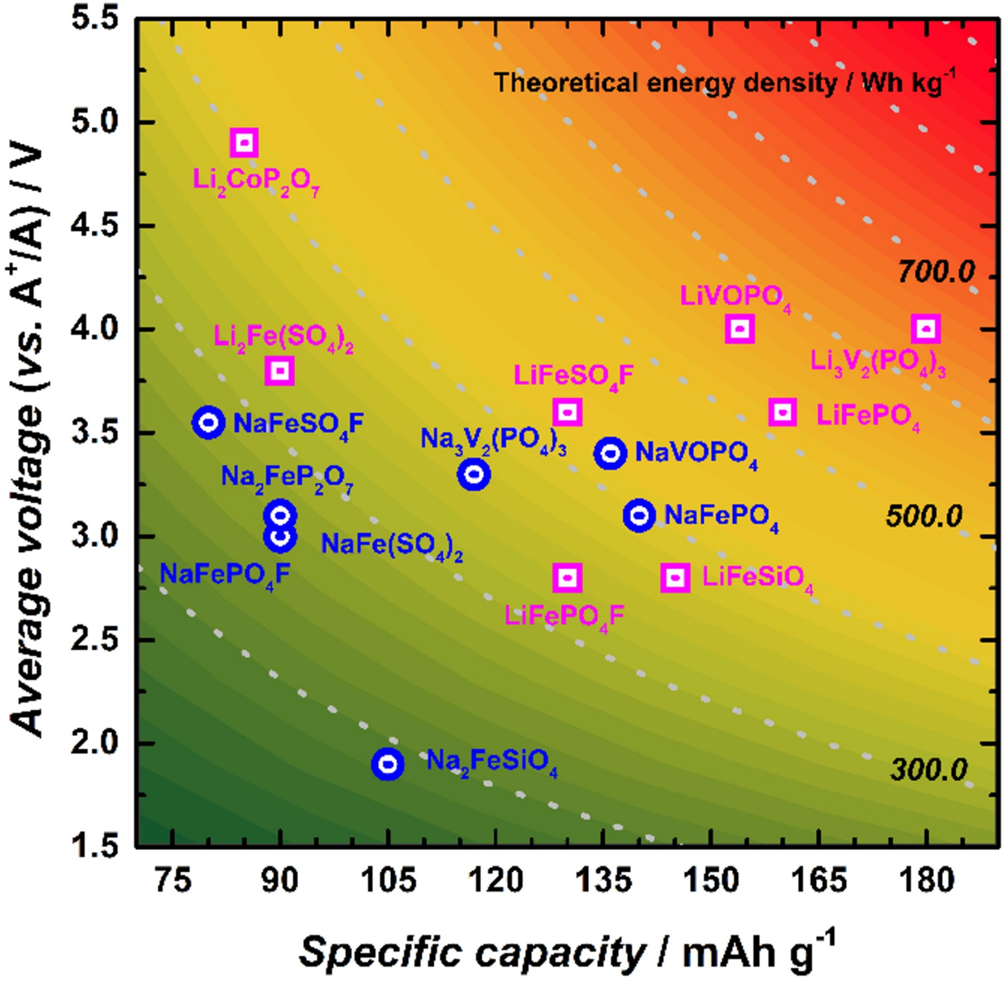
Tygesen, Chang, Vegge, Garcia-Lastra, npj Comp. Mater. 6, 1-9 (2020); Chen et al., J. Mater Chem A 8, 16551 (2020)

Li, Bhaghavathi, Vinayan, Jankowski, Njel, Roy, Vegge, Maibach, Lastra, Fichtner, Zhao-Karger, Angew. Chemie 59, 2 (2020)

Na-ion: Lower cost and more abundant

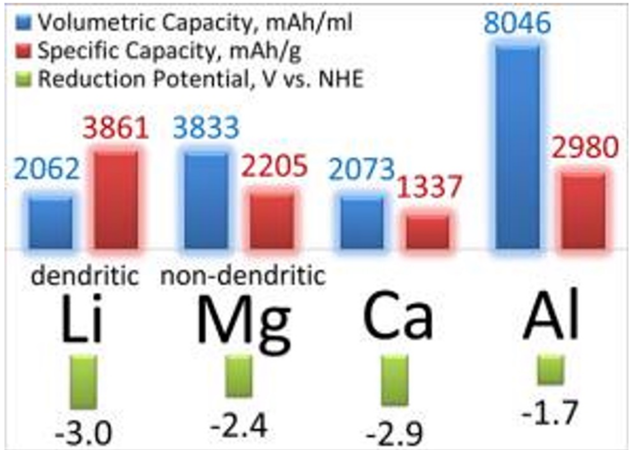
- Sodium ion batteries: utilizing Na^+ instead of Li^+
- CATL is now mass-producing gen 1 Na-ion (40 GWh) per year capacity



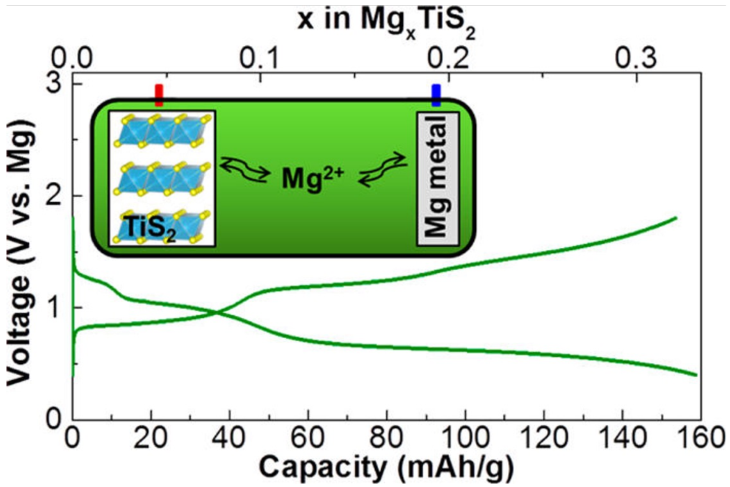


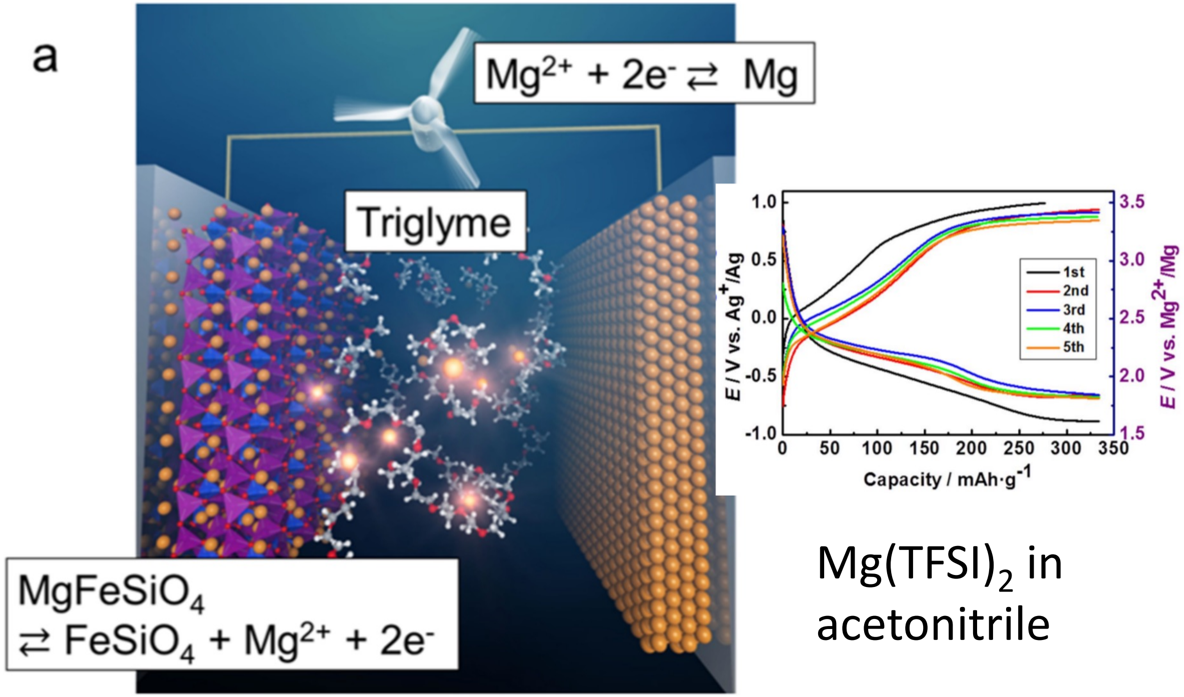
Nayak, P. K.; Yang, L.; Brehm, W.; Adelhelm, P. From Lithium-Ion to Sodium-Ion Batteries: A Materials Perspective. Angew. Chem. Int. Ed. , doi: 10.1002/anie.201703772.

Multivalent Metal Ion Batteries



Mg and Ca does not suffer from the same dendrite formation problem as Li does.





$Mg(TFSI)_2$ in acetonitrile

Large overpotentials

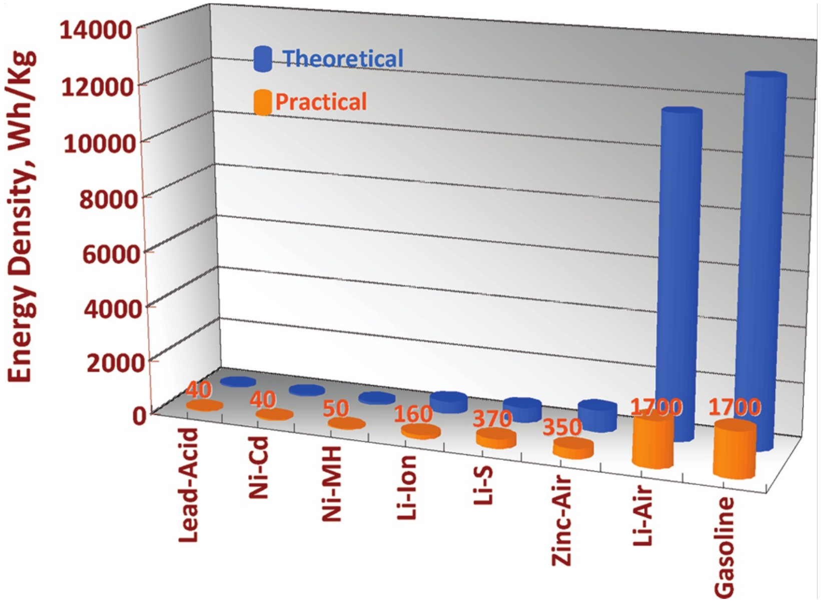
Capacities over 300 mAh/g achieved

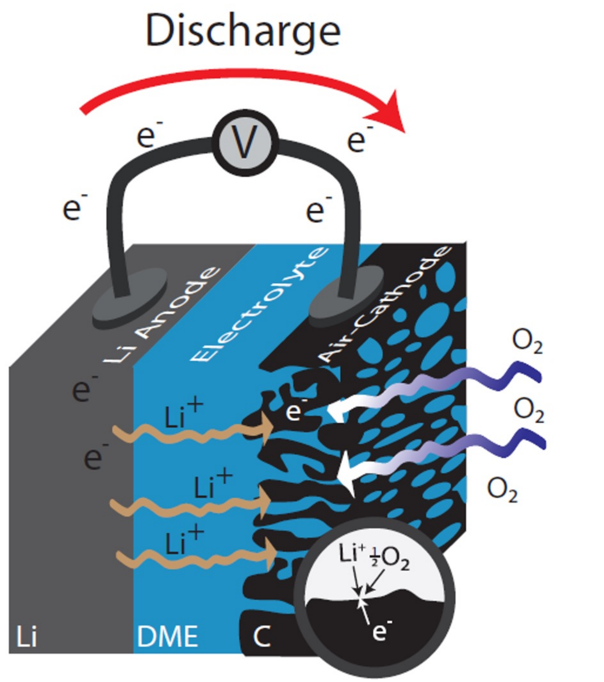
Sources:

Scientific Reports 2014, 4 DOI: 10.1038/srep05622 & Chem. Rev. 2014, 114 (23), 11683–11720 DOI: 10.1021/cr500049y & ACS Energy Lett. 2016, 1 (1), 297–301 DOI: 10.1021/acsenergylett.6b00145.

Metal-Air Cells

- The Li-Air battery utilizes the oxygen in ambient air, (largely) omitting heavy transition metals used in Li-ion batteries
- Reversible charge storage chemistry relying on the reversibility of lithium peroxide (Li_2O_2)
- Results in a potentially significant increase energy density



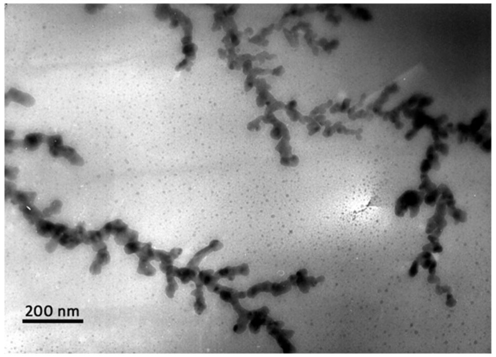


Sources:

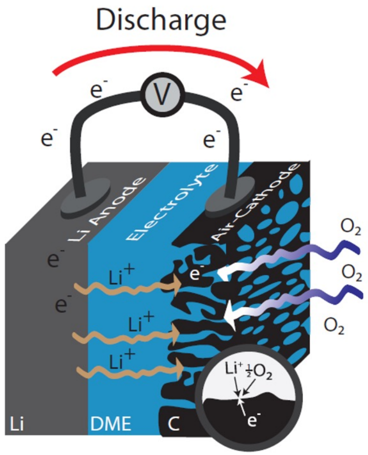
1.K. M. Abraham, Z. Jiang; *J. Electrochem. Soc.*, 143, 1 (1996).

2. G. Girishkumar, B. McCloskey, A. C. Luntz, S. Swanson, and W. Wilcke, *J. Phys. Chem. Lett.*, 1, 2193–2203 (2010).

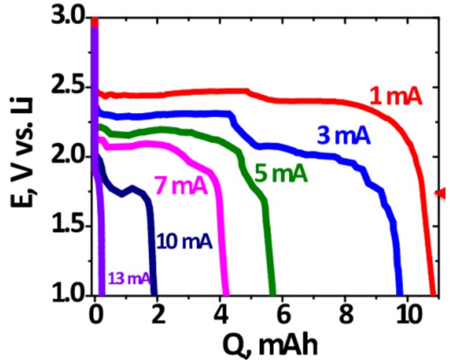
Li-Air Cells – Main Challenges



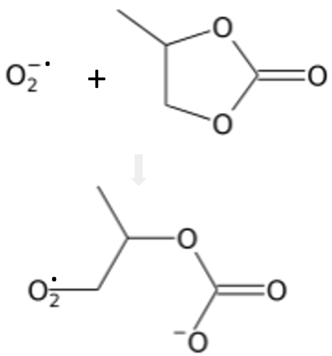
Dendrite formation

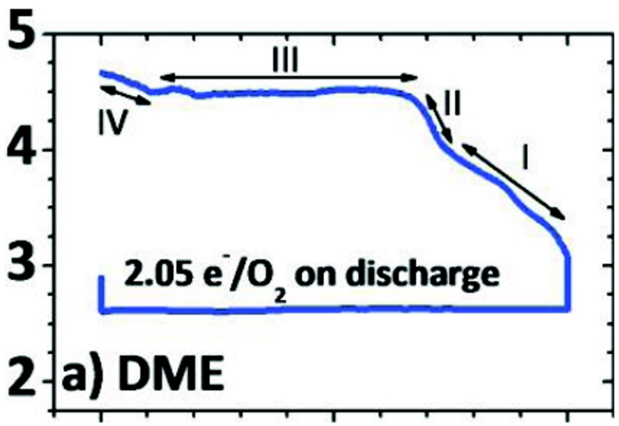


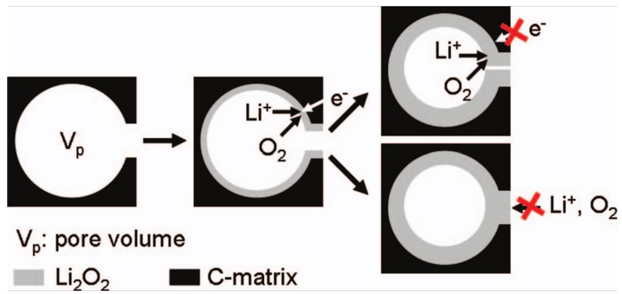
Poor rate capability



Poor electronic conductivity of Li_2O_2







Solvent Stability

J. Phys. Chem. A, 115, 12399–12409 (2011)

High Overpotentials

J. Phys. Chem. Lett., 2, 1161–1166 (2011).

Limited Capacity

J. Electrochem. Soc., 159, R1 (2012)

From e-mobility to Grid-Scale Storage

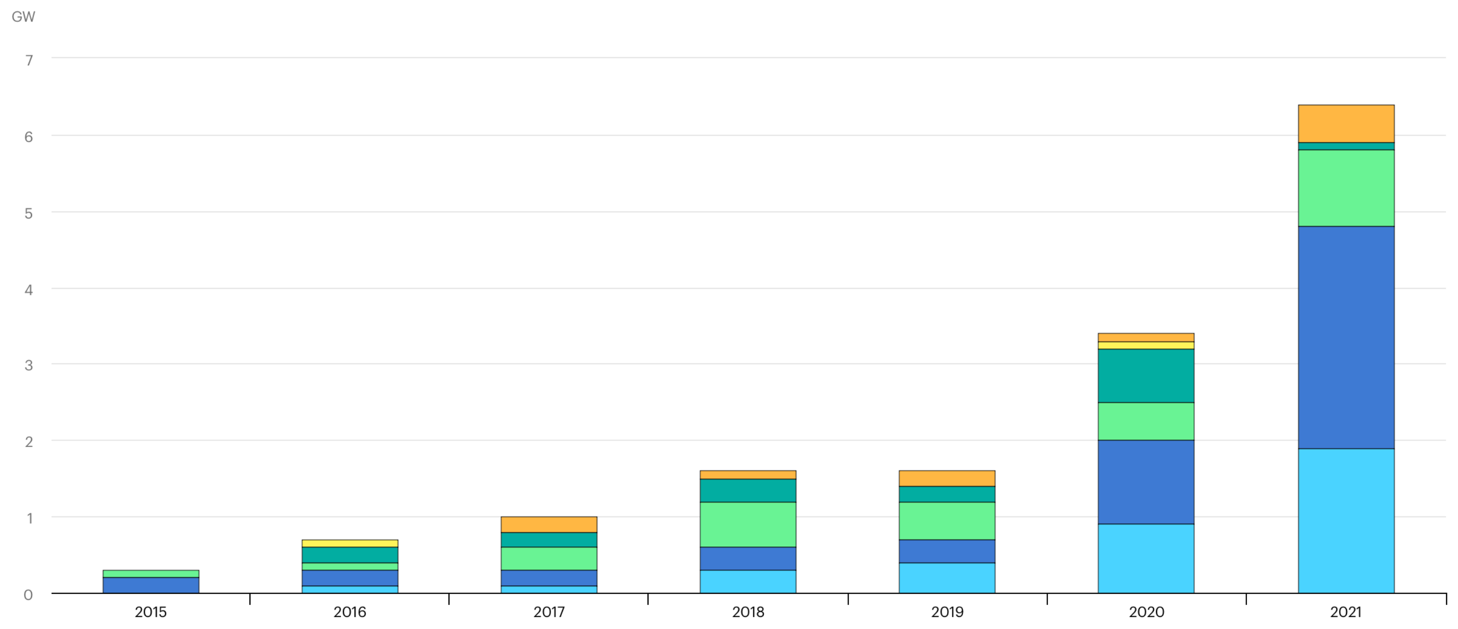
- Li-ion batteries hold potential for household storage, as well as short-term, grid-scale storage (100MW/129MWh)
- Stationary/grid-scale storage opens for alternative battery concepts and technologies

Tesla Energy – Powerwall 2 og Tesla's Hornsdale batteriinstallation (2017)

Annual new grid-installations (batteries)

- Still small compared to the transportation sector, but growing faster

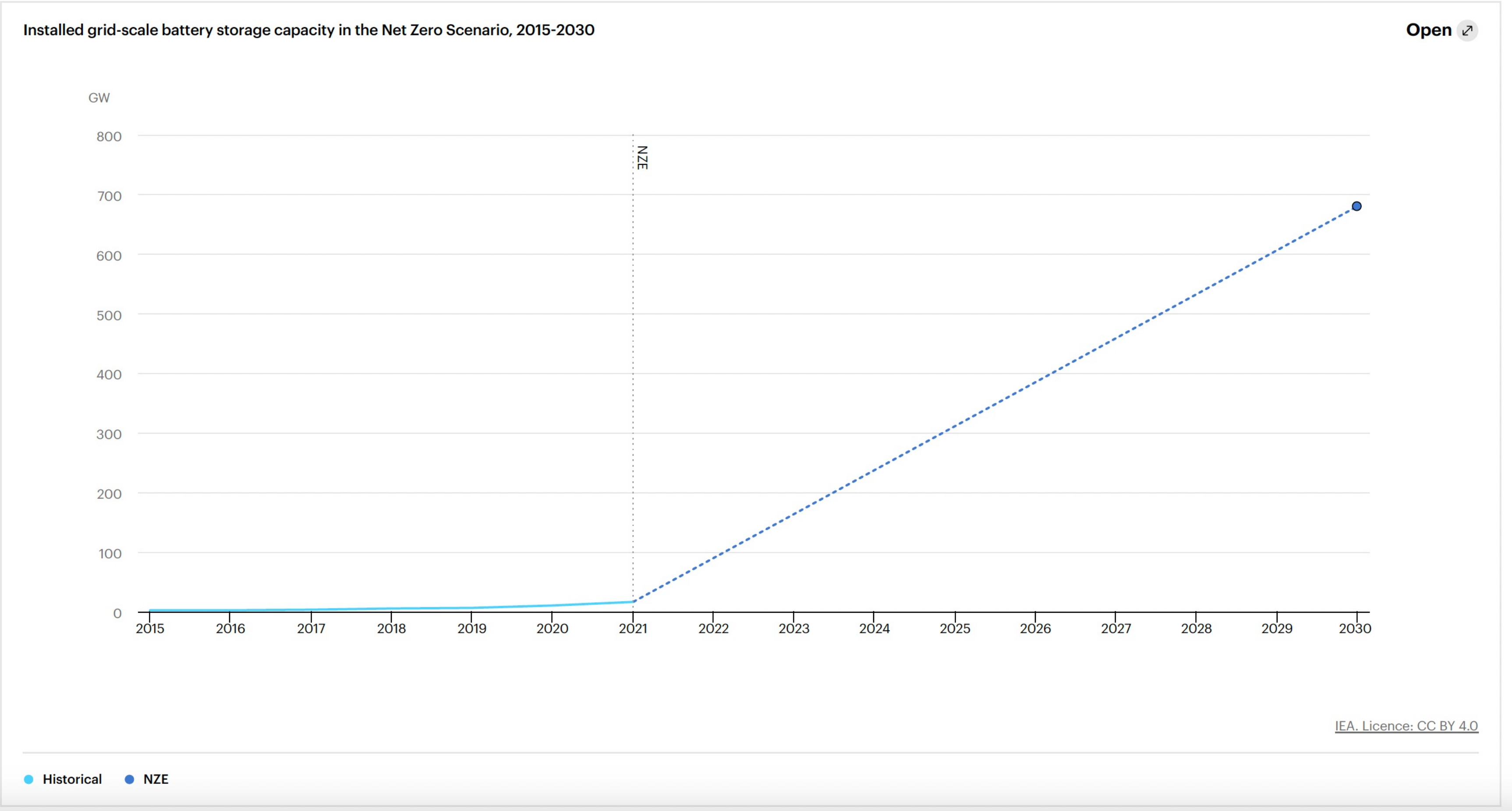
Download chart ↓ Cite Share



IEA Grid-Scale Storage (2022)

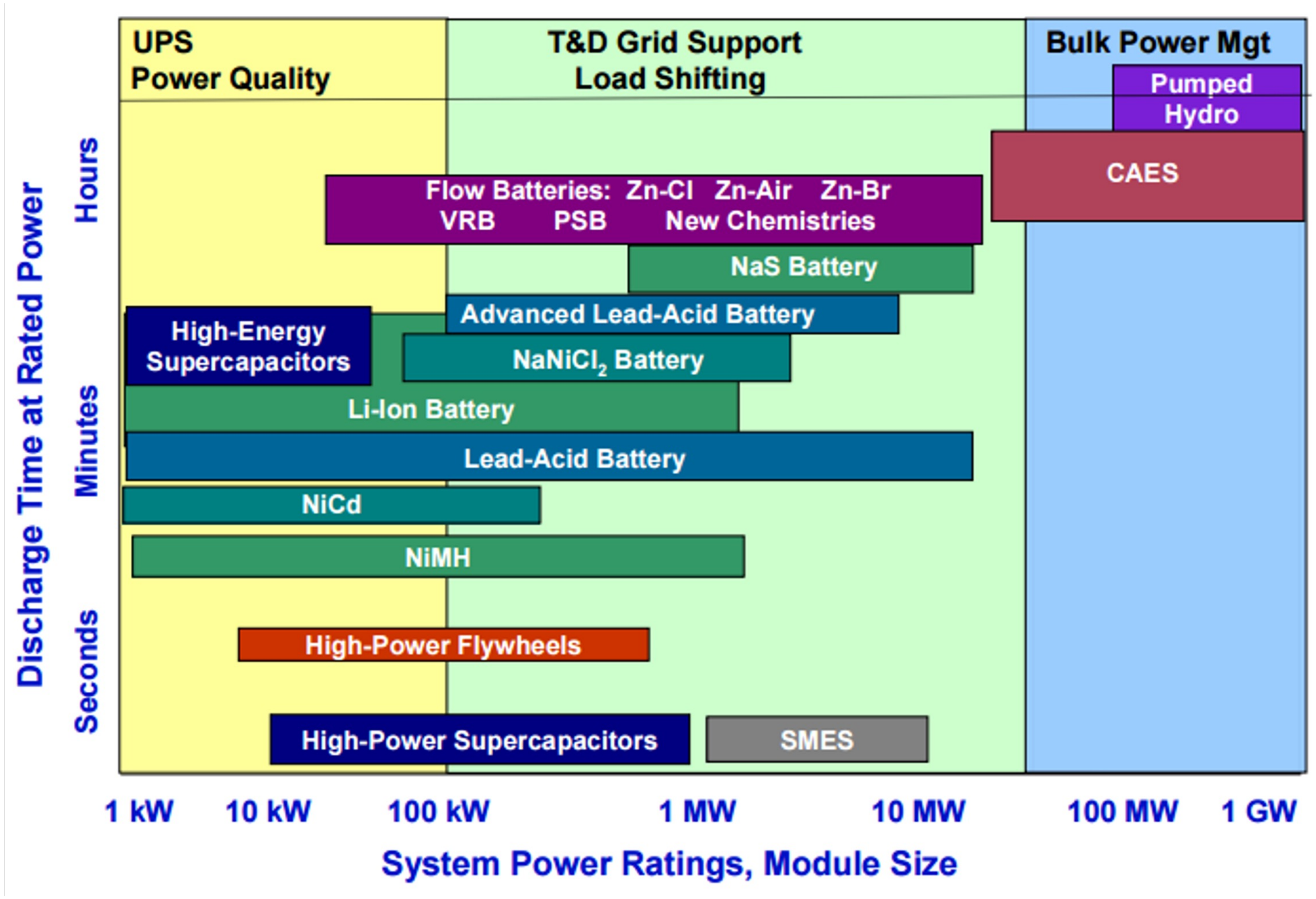
Annual new grid-installations (batteries)

- Installed battery capacity need in the Net Zero Scenario



IEA Grid-Scale Storage (2022)

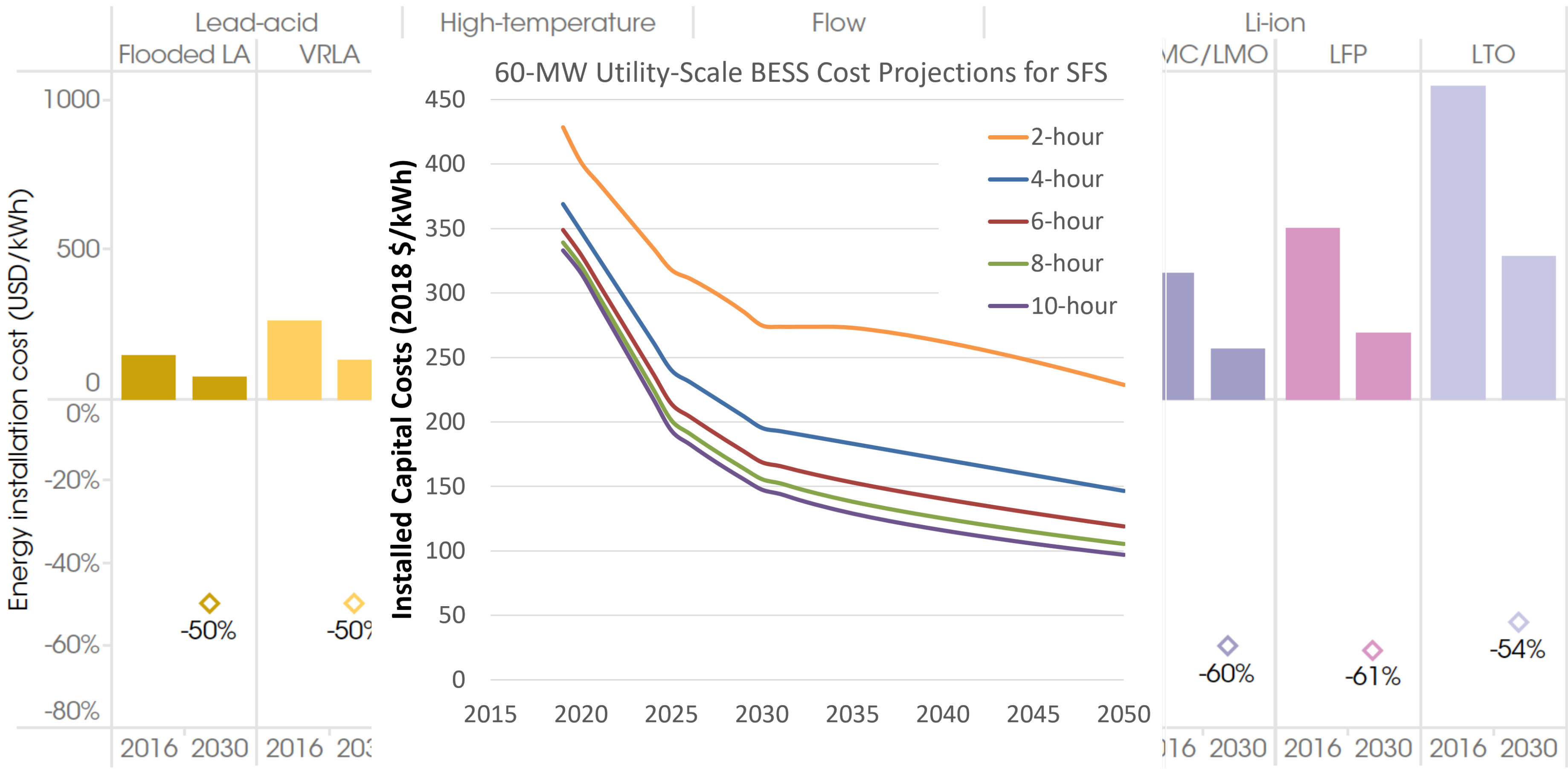
Energy Storage Technologies - Overview



Source: DOE/EPRI 2013 Electricity Storage Handbook in Collaboration with NRECA, SAND2013-5131

Installed cost

Figure ES6: Battery electricity storage system installed energy cost reduction potential, 2016-2030

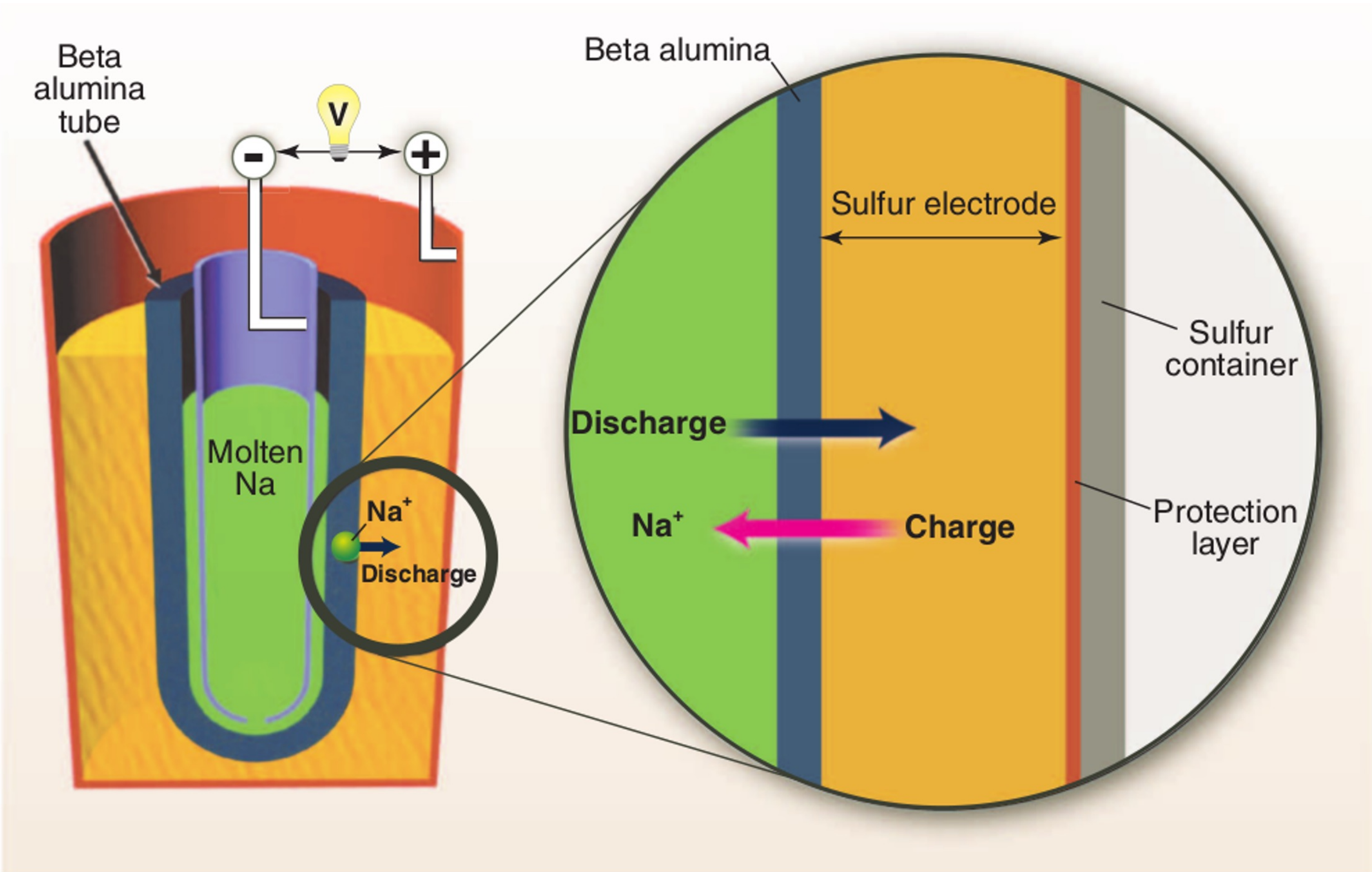


Note: LA = lead-acid; VRLA = valve-regulated lead-acid; NaS = sodium sulphur; NaNiCl = sodium nickel chloride; VRFB = vanadium redox flow battery; ZBFB = zinc bromine flow battery; NCA = nickel cobalt aluminium; NMC/LMO = nickel manganese cobalt oxide/lithium manganese oxide; LFP = lithium iron phosphate; LTO = lithium titanate.

IRENA, Electricity Storage and Renewables: Costs and Markets to 2030 (2017)
NREL Storage Futures Study (2022)

Metal-Sulfur Batteries

A high temperature battery ($T_{operation}$ = 200-300 °C) employing a solid Na-ion conducting electrolyte and the very low cost (and highly abundant) materials sodium and sulfur.



Source: Dunn et al; Electrical Energy Storage for the Grid: A Battery of Choices. Science 2011, 334 (6058), 928–935 DOI: 10.1126/science.1212741.

Sodium – Sulfur (Na-S) Battery Installations

Image: NGK, Buzen installation, 50 MW, 300 MWh (6 hours storage)

Initial report on fire at 2MW installation at Tsukuba Plant : http://www.ngk.co.jp/english/news/2011/0922.html
Report on cause of fire and resumed operation: http://www.ngk.co.jp/english/news/2012/0607.html

Flow Batteries for Energy Storage

- Flow batteries have <u>independently scalable Energy and Power</u> ratings:

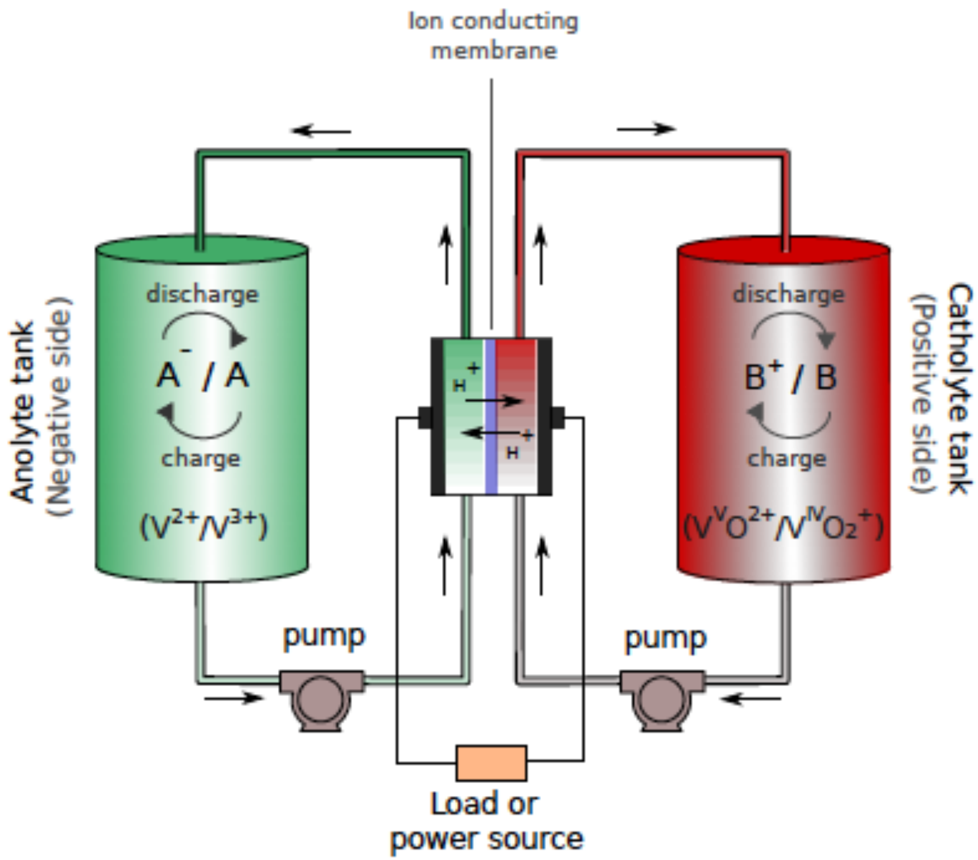
→ Storing **more energy** simply requires bigger electrolyte tanks

→ Increasing the **power** is done by increasing the electrode area

- Thus, the Energy / Power ratio is a design parameter: it can be tuned to the application!

- Fast response times

- Can be used for most energy services (sub-second → hours → days)



Negative side: $V^{3+} + e^- \underset{\text{discharge}}{\overset{\text{charge}}{\rightleftarrows}} V^{2+}$

Positive side: $VO_2^+ + e^- + 2H^+ \underset{\text{charge}}{\overset{\text{discharge}}{\rightleftarrows}} VO^{2+} + H_2O$

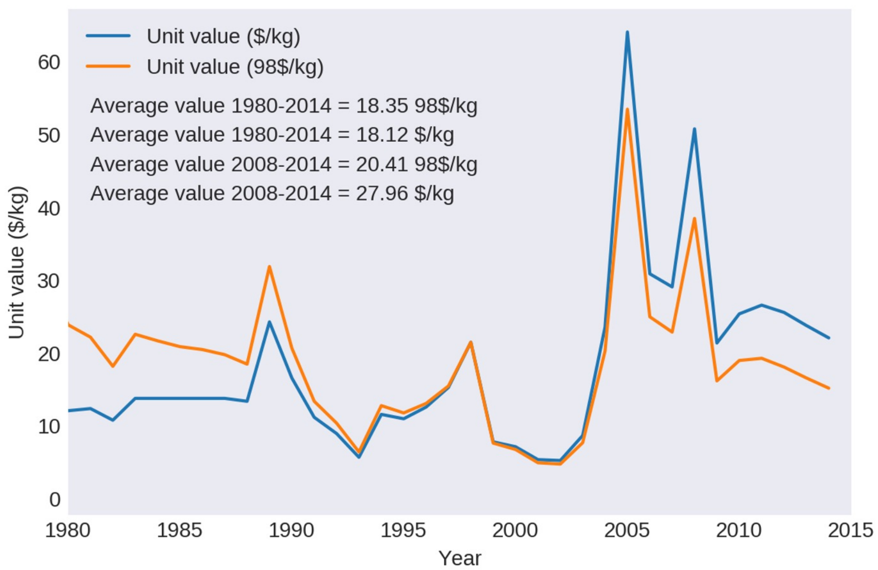
Main Flow Battery Chemistries

System	Reactions	E_{cell}^{o}	Electrolyte
Redox			Anode/Cathode
All Vanadium [3]	Anode: $V^{2+} \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} V^{3+} + e^-$ Cathode: $VO_2^{+} + e^- \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} VO^{2+}$	1.4 V	H_2SO_4/H_2SO_4
Vanadium-Polyhalide [5]	Anode: $V^{2+} \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} V^{3+} + e^-$ Cathode: $\frac{1}{2} Br_2 + e^- \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} Br^-$	1.3 V	VCl_3-HCl/NaBr-HCl
Bromine-Polysulfide [6]	Anode: $2\,S_2^{2-} \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} S_4^{2-} + 2e^-$ Cathode: $Br_2 + 2e^- \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} 2\,Br^-$	1.5 V	$NaS_2/NaBr$
Iron-Chromium [7]	Anode: $Fe^{2+} \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} Fe^{3+} + e^-$ Cathode: $Cr^{3+} + e^- \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} Cr^{2+}$	1.2 V	HCl/HCl
H_2-Br_2 [8]	Anode: $H_2 \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} 2H^{+} + 2e^-$ Cathode: $Br_2 + 2e^- \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} 2Br^-$	1.1 V	PEM*- HBr
Hybrid			
Zinc-Bromine	Anode: $Zn \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} Zn^{2+} + 2e^-$ Cathode: $Br_2 + 2e^- \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} 2\,Br^-$	1.8 V	$ZnBr_2/ZnBr_2$
Zinc-Cerium [9]	Anode: $Zn \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} Zn^{2+} + 2e^-$ Cathode: $2Ce^{4+} + 2e^- \xleftarrow{\text{charge}}\xrightarrow{\text{discharge}} 2Ce^{3+}$	2.4 V	CH_3SO_3H (both sides)

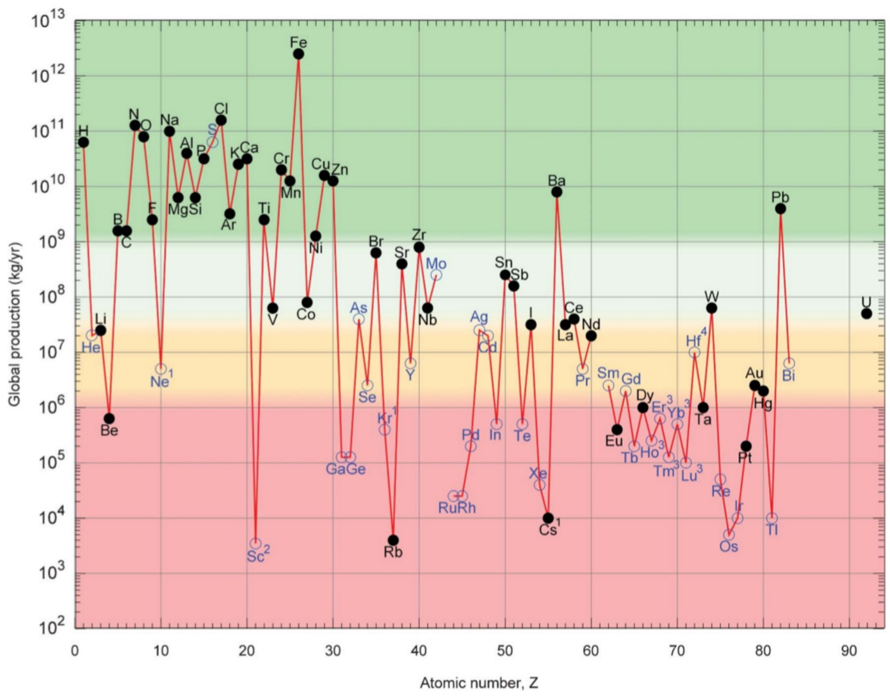
The State of Art: Vanadium Flow Batteries

•The most commonly researched and commercialized type of flow battery relies on the use of vanadium ($V^{II/III}$,$V^{IV/V}$) as the charge storage medium.

•BUT: **Vanadium is expensive**, has displayed significant price volatility, and is a limited natural resource!



Cost of vanadium (2008-2014): ~$85 / kWh



Vanadium redox flow batteries (VRB)

Dalian, Kina, 100MW/400MWh VRB (2022)

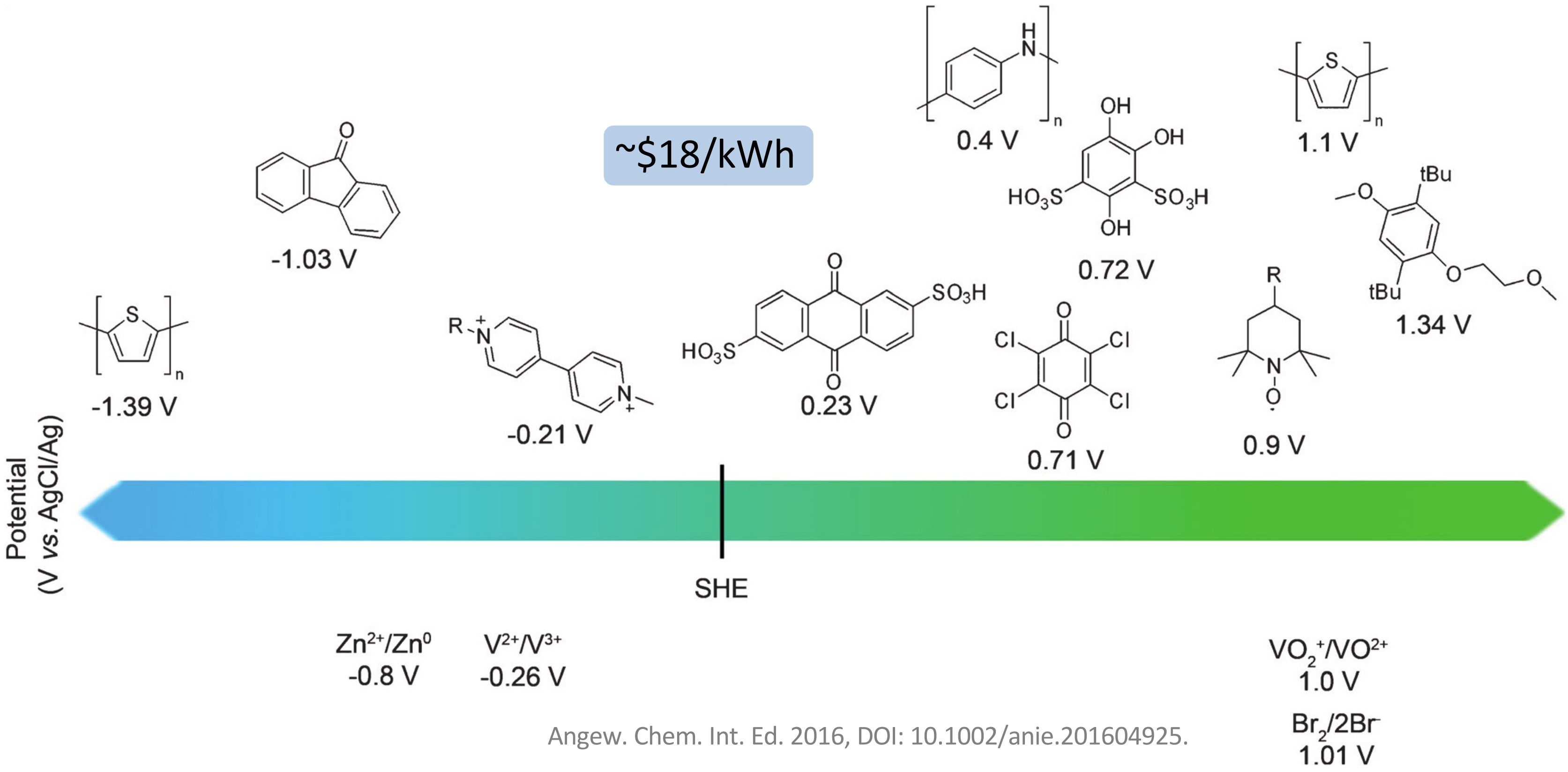
Organic Flow Batteries

- Interest in Organic Flow Batteries mainly driven by two things:

→ The pursuit of lower cost energy storage solutions (CAPEX < $100/kWh)

→ Sustainability of truly large scale energy storage (Utilizing only abundant elements)

- Utilizing reversible redox reactions of organic compounds



Angew. Chem. Int. Ed. 2016, DOI: 10.1002/anie.201604925.

Batteries – Summary and Outlook

- Highly efficient (rechargeable) devices for electrochemical energy storage
- Energy/power density, safety/durability and cost remain critical factors
- Battery technologies plays a key role in the international transition to renewable energy, e.g. in the transportation sector and for household and utility/grids scale storage on short-to-medium time-scales
- Traditional Li-ion chemistries, e.g. NMC and LFP, will likely continue to dominate over the next +5 years, but NMC-type may ultimately be limited by their scarce metals
- Alternatives like all solid-state batteries and Na-ion will play an increasing role over the next 5 years
- A large-scale introduction of batteries for energy storage must rely on more earth-abundant metals and/or organic materials
- The development of next-generation battery technologies will likely be driven by regions that unite information technology, e.g., Big Data and materials-by-design, car producers and the chemical industry (see www.big-map.eu)