SIMBA materials development
AB 1st Workshop

21 July 2022

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KIT-HIU

This project has received funding from the European Commission under grant agreement No 963542

Three Working groups

- Leading questions Working groups
  - How do you compare the SIMBA materials and cell development with the current SoA for stationary storage batteries?
  - What steps are still needed to make SIMBA Na-ion technology even more promising?
  - What does the end user, policymaker requests from Na-ion technology batteries for stationary storage applications? (Pathways to Impact)

	SIMBA material development	SIMBA cell development	SIMBA safety, standards and recycling steps
SoA stationary storage batteries			
Challenges Na technology			
Future pathways - Impact			

SIMBA project: Concept

+SIMBA
SODIUM-ION AND SODIUM METAL BATTERIES

Main goal

Development of a **highly cost-effective**, **safe**, **all-solid-state battery** with **sodium** as a mobile ionic charge carrier for **stationary storage applications**

Option 1

Hard carbon (TRL5)

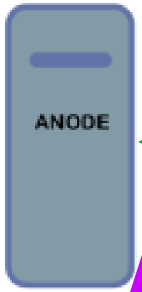
- Sustainable sources
- High capacity (280 mAh g^{-1})

Option 2

Porous ceramic structure

- Support for Na plating
- High specific capacity (> 500 mAh g^{-1})

Aluminum substrate

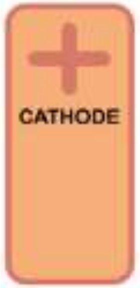


Na+

Solid state electrolyte (SSE) (TRL3-5)

- Single-ion conductive polymers
- Optimized safe Na-ion transport
- Stability window up to 4.4 V
- Ionic conductivities of 10^{-3} S cm^{-1} at RT

Na+



Option 1

Iron-based Prussian White (TRL5)

- Ultra low-cost (< 4 € kg^{-1})
- Good capacity (165 mAh g^{-1})
- Acceptable working voltage (3 V)
- Scalable

Option 2

2nd Gen: layered oxide (TRL5)

- High energy material (> 200 mAh g^{-1} and > 3 V)

Aluminum substrate

New modelling and characterization tools

- Deep understanding of interface kinetics and degradation mechanism
- Design optimal chemical interface

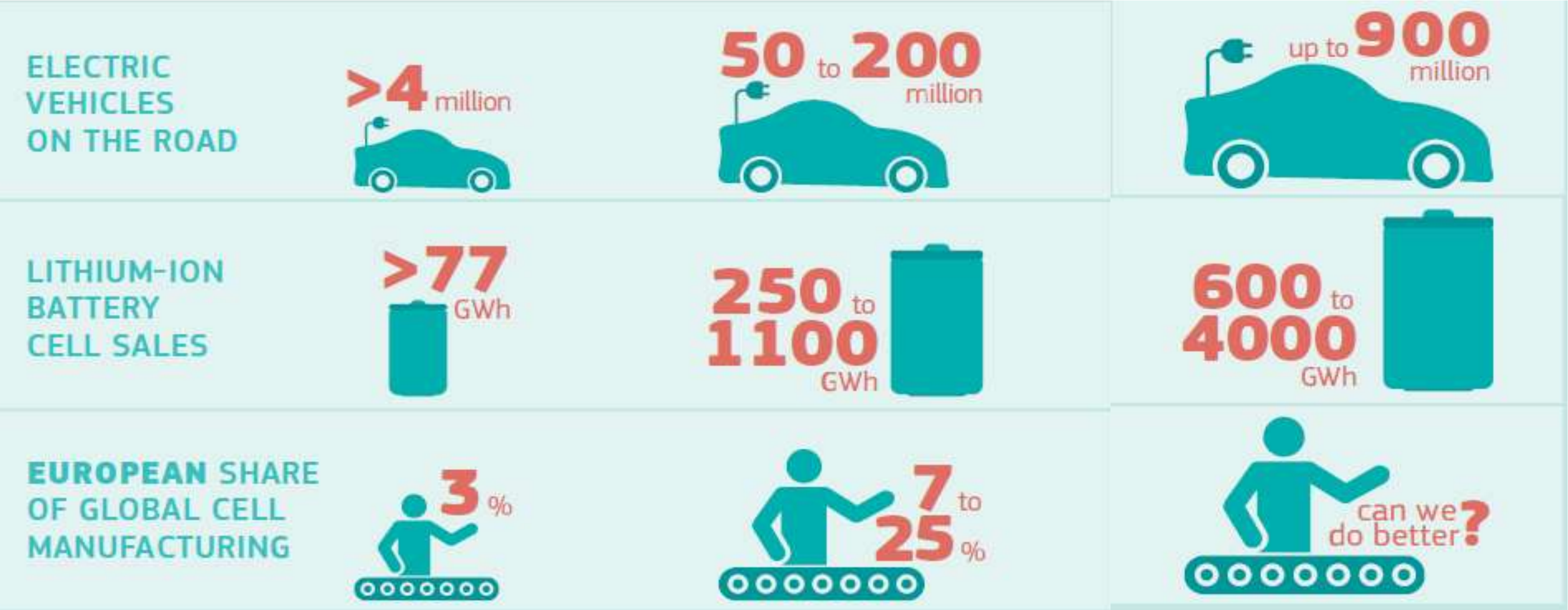
Two sustainable electrode production processes

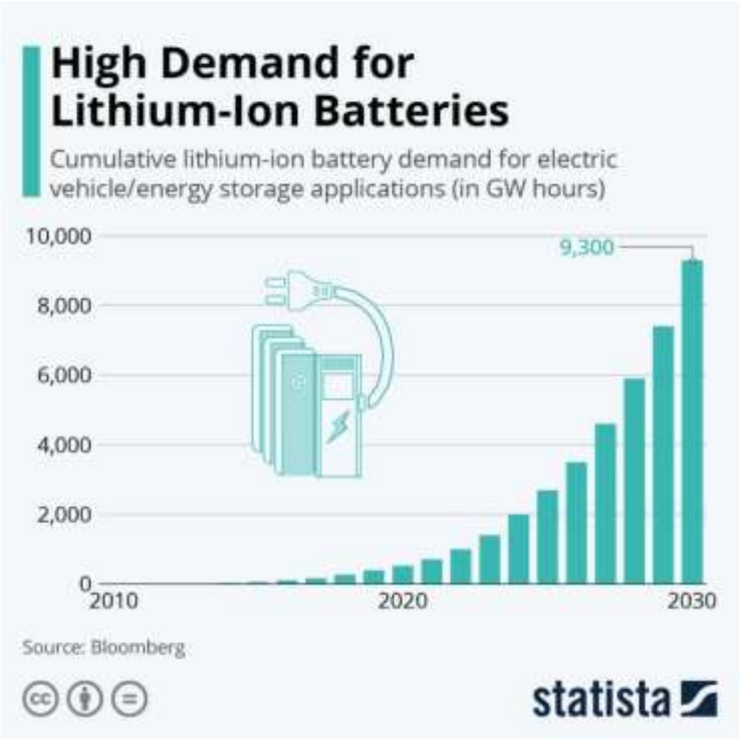
- Water-based binder
- Extrusion solvent free

Scenario of Lithium-ion batteries

Global supply and demand of Lithium-ion batteries today and in the future

2018 **2028** **2040**





...but Lithium-ion batteries show environmental and societal challenges associated with their mass production

https://ec.europa.eu/jrc/sites/default/files/jrc114616_li-ion_batteries_two-pager_final.pdf
https://www.statista.com/chart/23808/lithium-ion-battery-demand/

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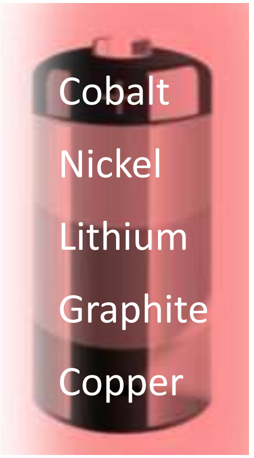
SODIUM-ION AND SODIUM METAL BATTERIES

Why sodium technology?

LIBs: dependency on critical materials



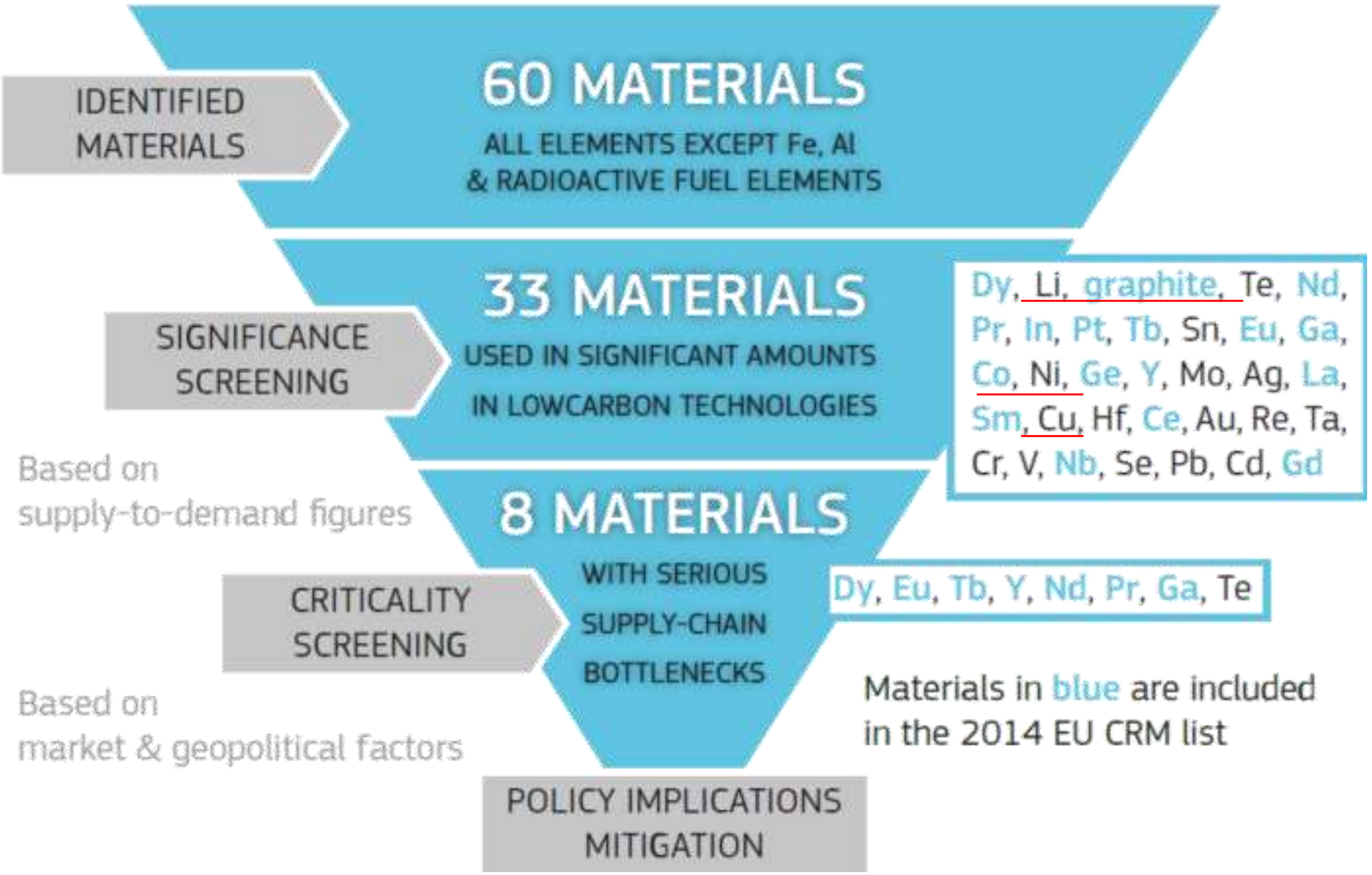
- ❑ Geopolitical supply risks
- ❑ Substitutability supply restrictions
- ❑ Environmental implications

Alternative low-cost, sustainable and more environmentally friendly EES

Sodium-ion batteries

Manganese
Iron
Hard Carbon
Sodium
Aluminum

Identification of critical materials for the EU



https://setis.ec.europa.eu/setis-reports/setis-magazine/materials-energy/critical-materials-energy-technologies-evangelos
I. Hasa et al. J. Power Sources (2021) 482, 228872

Sodium-prototypes

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SODIUM-ION AND SODIUM METAL BATTERIES

2013

Sharp Laboratories of America, Inc.
Anode: hard carbon
Cathode: Prussian White

Sumitomo Chemical Co. Ltd.
Anode: hard carbon
Cathode: O3- Mn/Fe/Ni layered oxide

2015

Faradion Ltd.
Anode: hard carbon
Cathode: O3-$Na_aNi_{(1-x-y-z)}Mn_xMg_yTi_zO_2$

2017

Sharp Laboratories of Europe, Inc.
Anode: hard carbon
Cathode: O3-$NaNi_{1/3}Fe_{1/6}Mn_{1/3}Mg_{1/12}Sn_{1/12}O_2$

Novasis Energies Inc.
Anode: hard carbon
Cathode: PBA

2018

RS2E/Tiamat
Anode: hard carbon
Cathode: V-phosphate

2019

HiNa Battery technology Co.
Anode: soft
Cathode: O3

HiNa Battery technology Co.
30 kW/100 kWh large-scale EES

2023

CATL
Na-ion/Li-ion one pack
Anode: hard carbon
Cathode: PW

Materials for SIBs:
Anode: hard carbon
Cathode: PW or layered oxides
Electrolyte: carbonate-based

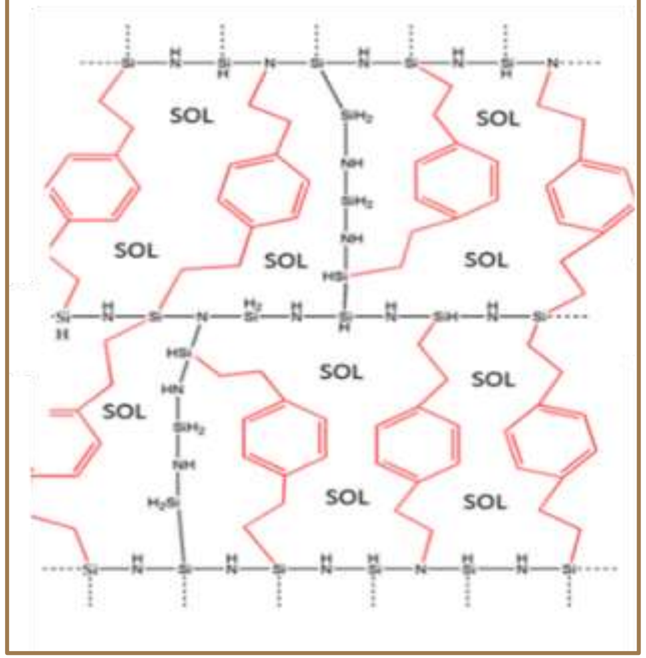
S. Kuze, et al. *R&D Report "SUMITOMO KAGAKU"* (2013) / A. Bauer et al. Adv. Energy Mater. (2018) 8, 1702869 / K. Smith et al. ECS Trans. (2017) 75, 13.
S. Kakimoto, et al. J. Am. Chem. Soc. (2015) 137, 2548 / https://news.cnrs.fr/articles/a-battery-revolution-in-motion / Y. Li et al. Energy Storage Mater. (2016) 5, 191.

SIMBA

SODIUM-ION AND SODIUM METAL BATTERIES

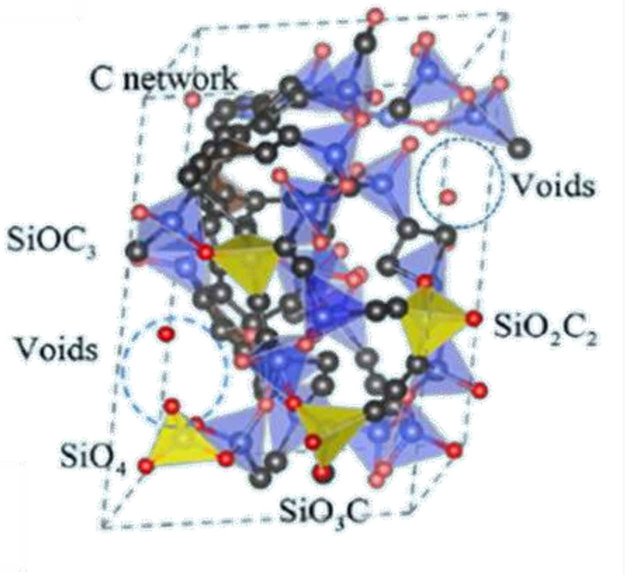
SIMBA anode materials

SiCN



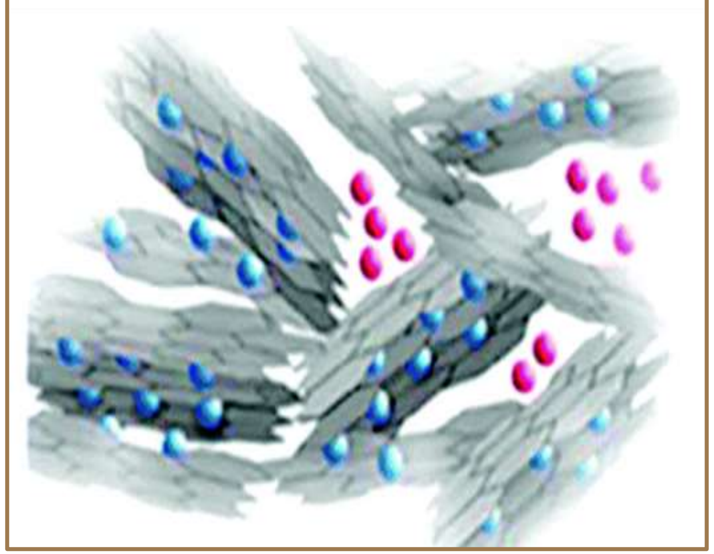
- Highly porous ceramic materials
- As Na plating matrix
- Sodium-metal batteries

SiOC



- Highly porous ceramic materials
- As Na plating matrix
- Sodium-metal batteries

Hard carbon

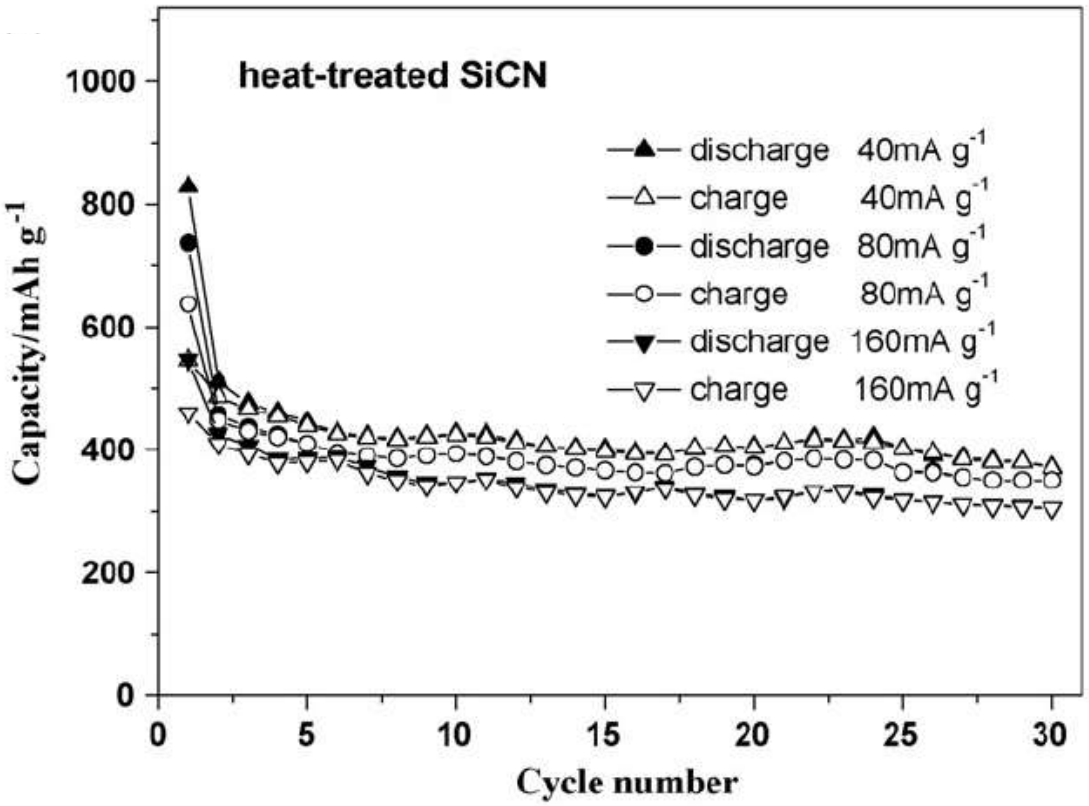


- Biowaste derived hard carbon
- Lignin-based precursors
- Sodium-ion batteries

Q. Wen, et al. J. Advanced Ceramics (2022) 11, 197-246
D. A. Stevens et al. J. Electrochem. Soc. (2000) 147, 1271–1273

SiCN: SoA

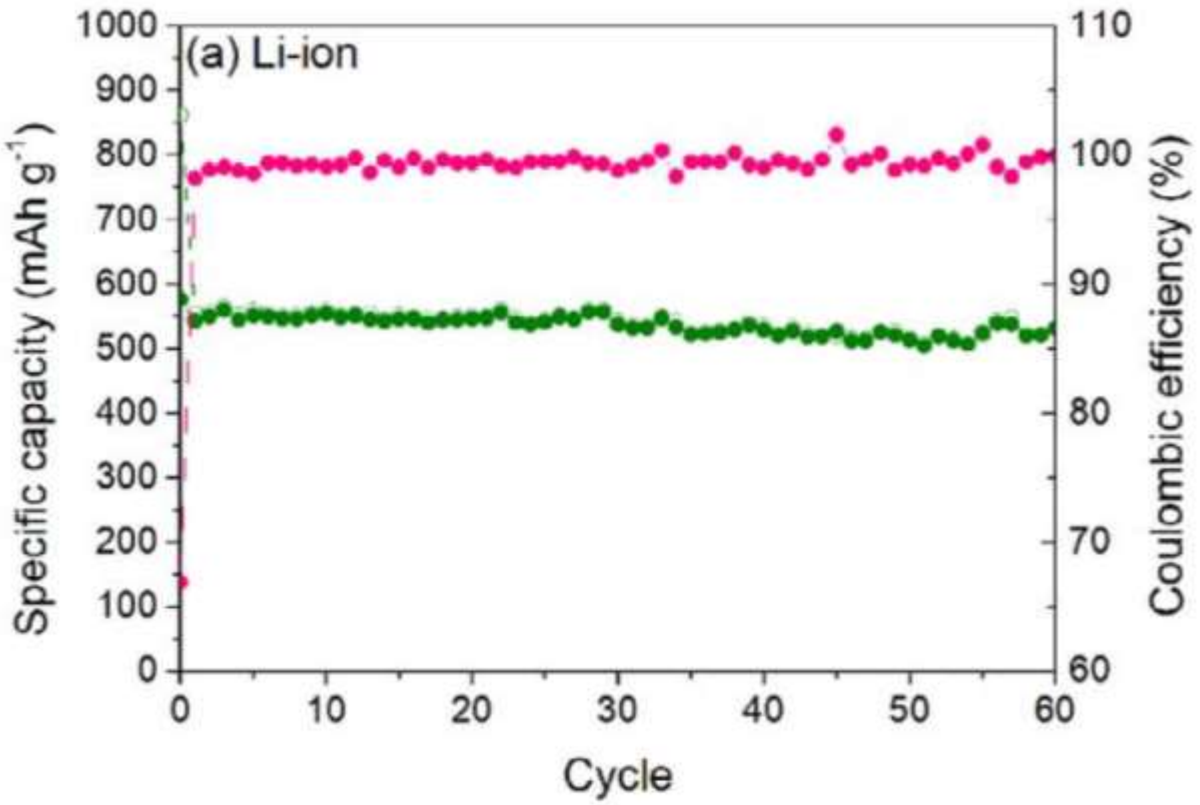
- **SoA:**
  - LIBs:
    - Precursor: polysilyethylendiamine at 1000-1300 °C
    - **Reversible specific capacity of 560 mAh g^{-1}**
    - ICE: 60.4%



Y. Feng, *Electrochimica Acta* (2010) 55, 5860–5866

SiOC: SoA

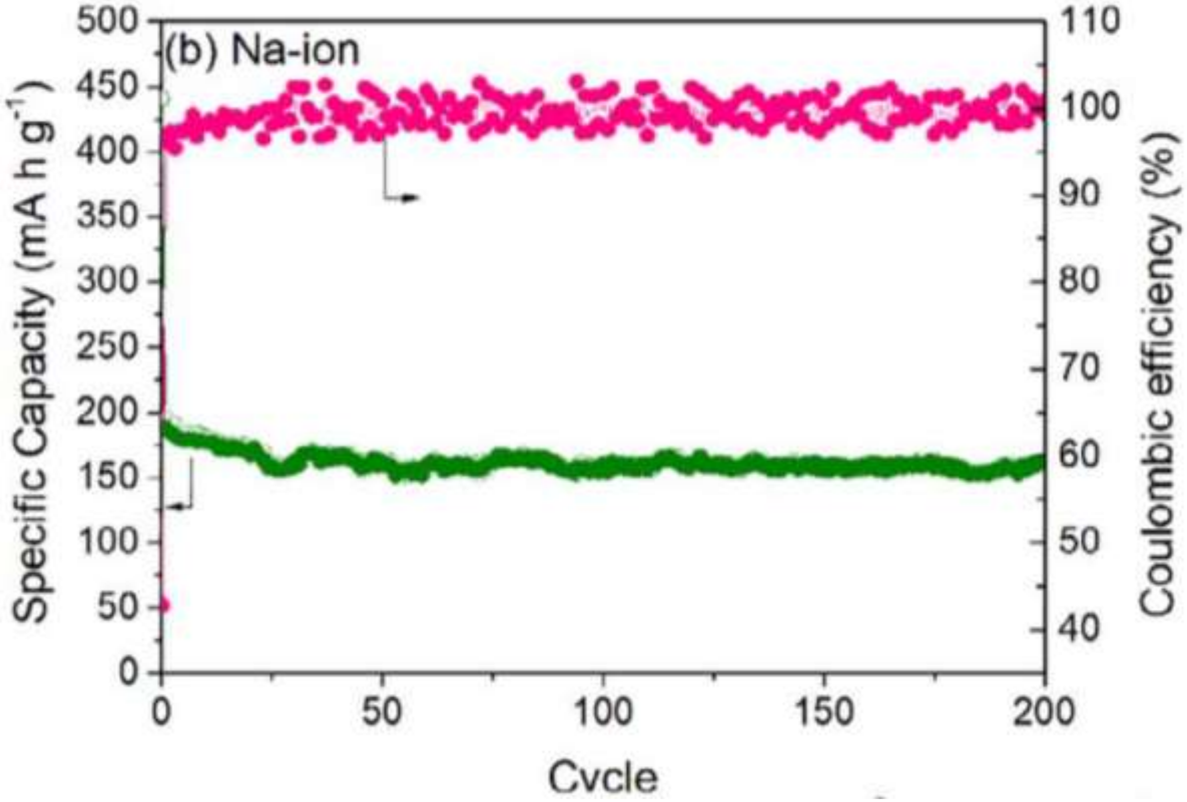
- **SoA:**
  - **LIBs:**
    - Precursor: silicone oil in H_2/Ar flow at 900 °C
    - **Reversible specific capacity of 550 mAh g^{-1}**
    - ICE: 67%
    - CE: ≈ 100% up to 60 cycles



Y. Feng, *Electrochimica Acta* (2010) 55, 5860–5866

SiCN: SoA

- **SoA:**
  - NIBs
    - Precursor: silicone oil in H_2/Ar flow **at 900 °C**
      - **Reversible specific capacity of 160 mAh g^{-1}** over 200 cycles
      - ICE: 43%
      - CE: fluctuating

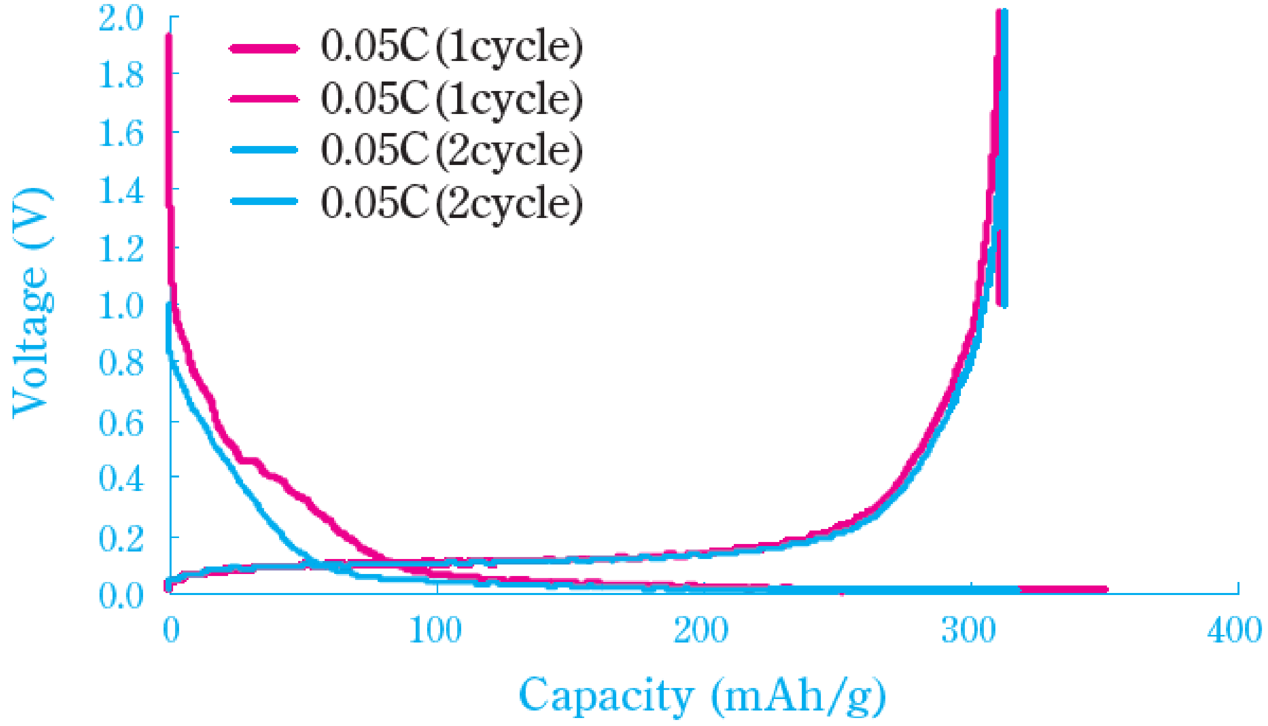


Y. Feng, *Electrochimica Acta* (2010) 55, 5860–5866

Hard carbon: SoA

- **SoA:**
  - Sumitomo Chemicals Co. Ltd.
    - Calixarenes derived hard carbon
    - **Reversible specific capacity of 320 mAh g^{-1}**
    - Excellent cycling
    - **ICE: 91%**

Electrolyte: 1M $NaPF_6$ in PC

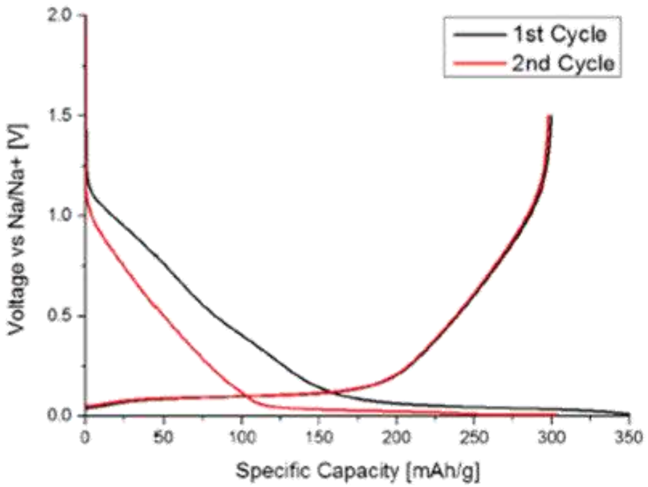


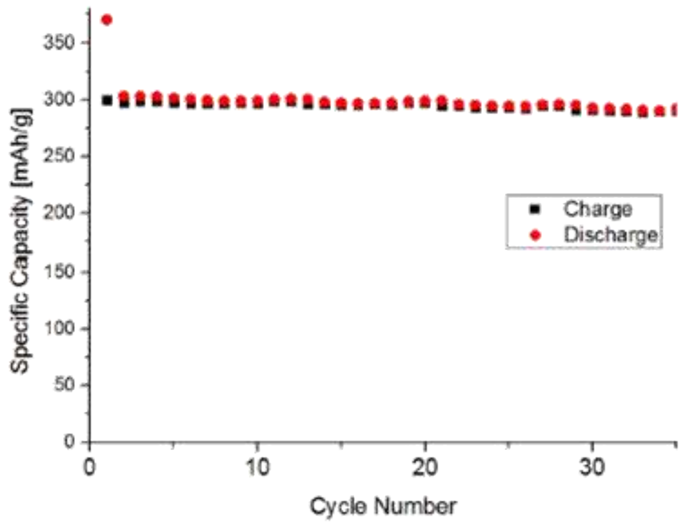
Hard carbon
O3- Mn/Fe/Ni layered oxide

S. Kuze, et al. *R&D Report "SUMITOMO KAGAKU"* (**2013**)

Hard carbon: SoA

- **SoA:**
  - Sharp Laboratories of Europe
    - Commercial hard carbon
    - Current collector: **C-Cu** or C-Al
    - Electrode formulation: 90:3.5:1.5:5 (AM:CB:MWCNT:PVdF)
    - Electrolyte: 1M $NaPF_6$ in EC:DEC (1:1)
    - **Reversible specific capacity of 300 mAh g^{-1}**
    - Excellent cycling
    - ICE: 82%





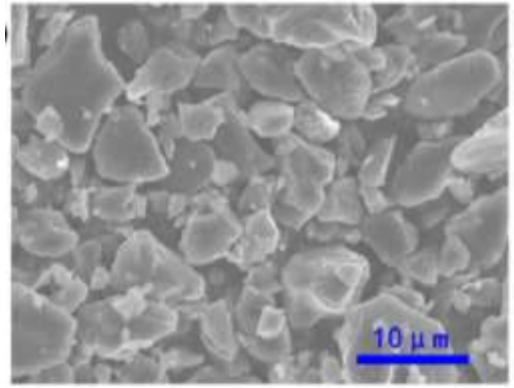
Hard carbon
$O3\text{-}NaNi_{1/3}Fe_{1/6}Mn_{1/3}Mg_{1/12}Sn_{1/12}O_2$

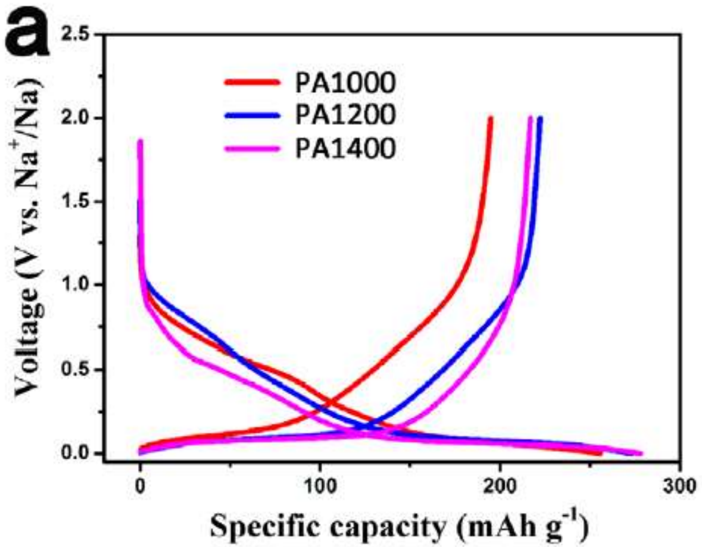
K. Smith, et al. ECS Trans. (2017) 75, 13.

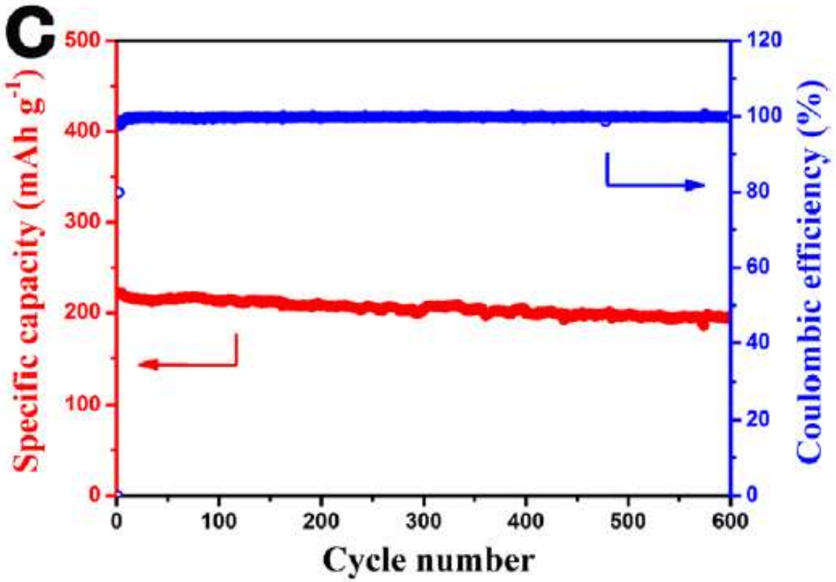
Hard carbon: SoA

- **SoA:**
  - HiNa Battery Technology Co.
    - Anthracite pyrolyzed soft carbon
    - Reversible specific capacity of 222 mAh g^{-1}
    - Excellent cycling (89% over 600 cycles at 0.2C)
    - Electrolyte: 0.8M $NaPF_6$ in EC:DMC (1:1vol%)
    - ICE: 81%

Soft carbon
O3 $Na_{0.9}Cu_{0.22}Fe_{0.30}Mn_{0.48}O_2$







Y. Li et al. Energy Storage Mater. (2016) 5, 191.

SIMBA cathode materials

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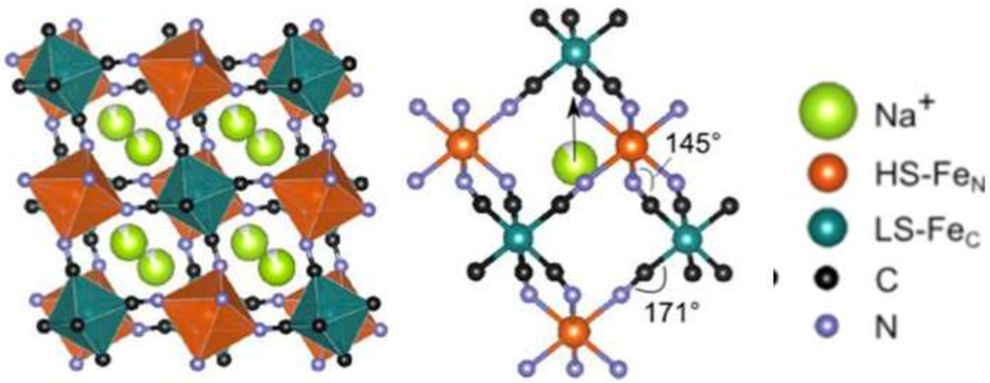
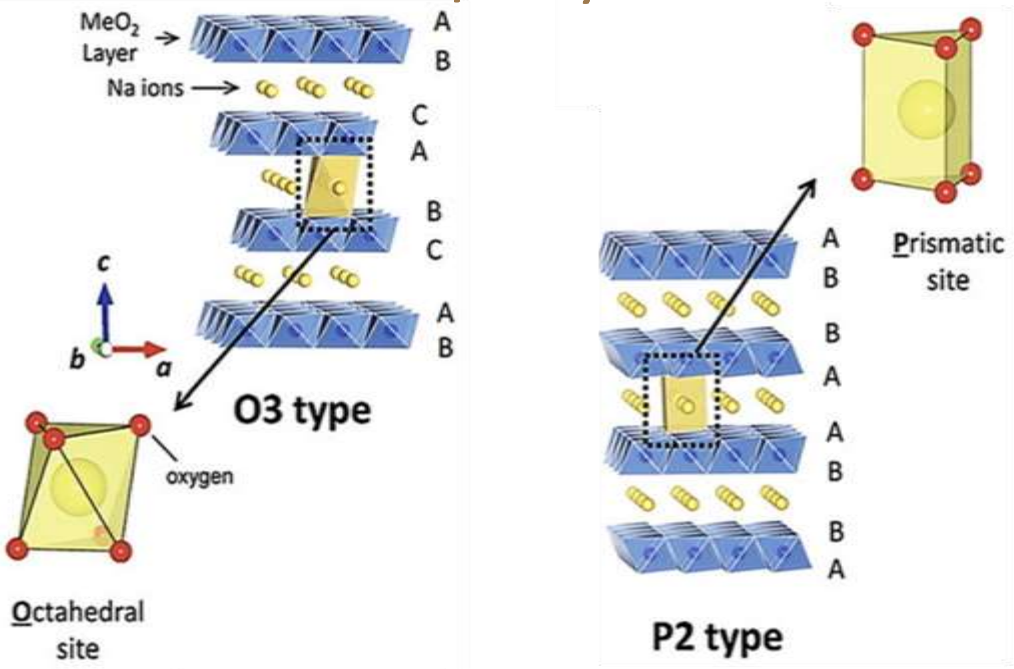
PBA - Prussian White



P2/O3 layered oxides



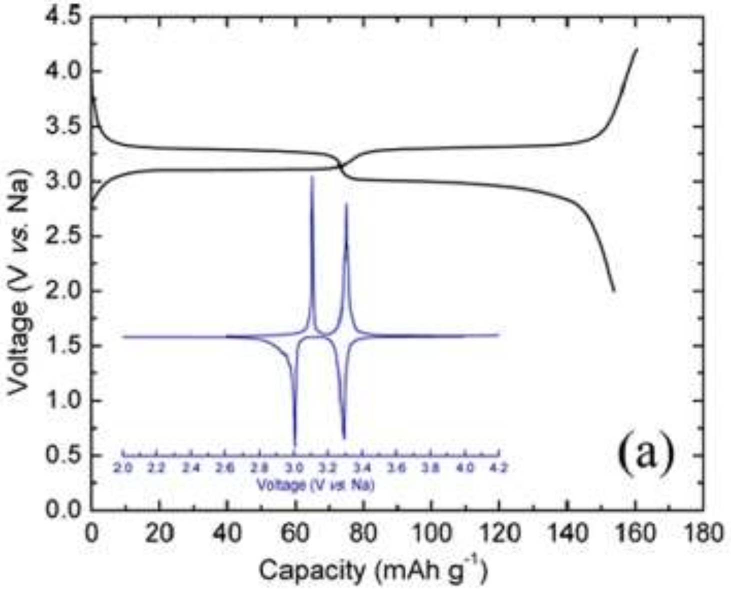
- Low-cost synthesis process
- Good capacity and acceptable average voltage

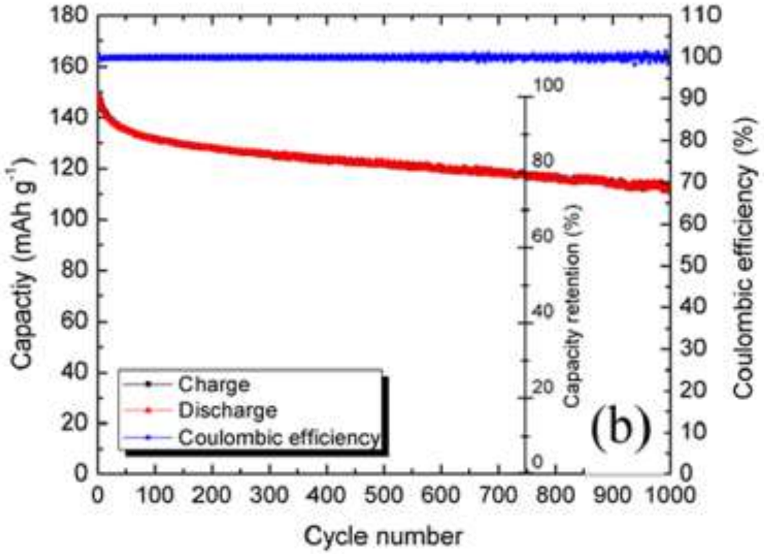
- Usually higher specific capacity

W. R. Brant, et al. Chem Mater (2019) 31, 7203-7211
K. Kubota, et al. MRS Bulletin (2014) 39, 416–422

Prussian White: SoA

- **SoA:**
  - Sharp Laboratories of America Inc.
    - Electrode formulation: 86:7:7 (PW:KB:PTFE)
    - Electrolyte: 1M $NaPF_6$ in EC:DEC (1:1vol%)
    - **1st charge capacity of 160 mAh g^{-1} (10 mA g^{-1})**
    - Cycling stability of 80% after 750 cycles



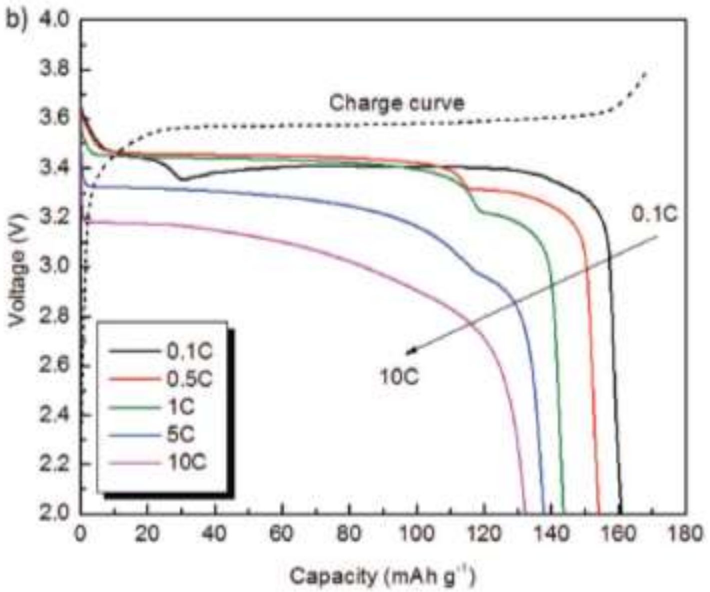


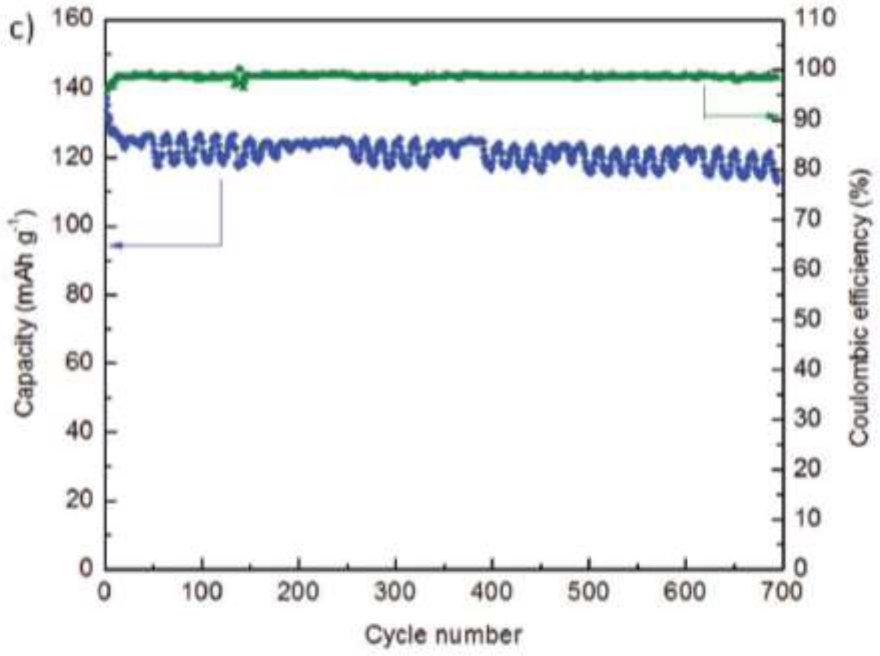
Hard carbon
Prussian White

L. Wang, et al. J. Am. Chem. Soc. 2015, 137, 2548.

Prussian White: SoA

- **SoA:**
  - Novasis Energies Inc.
    - Specific discharge capacity from 160 to 132 mAh g^{-1} (from 0.1 to 10C)
    - Stable cycling performance at 1C over 700 cycles





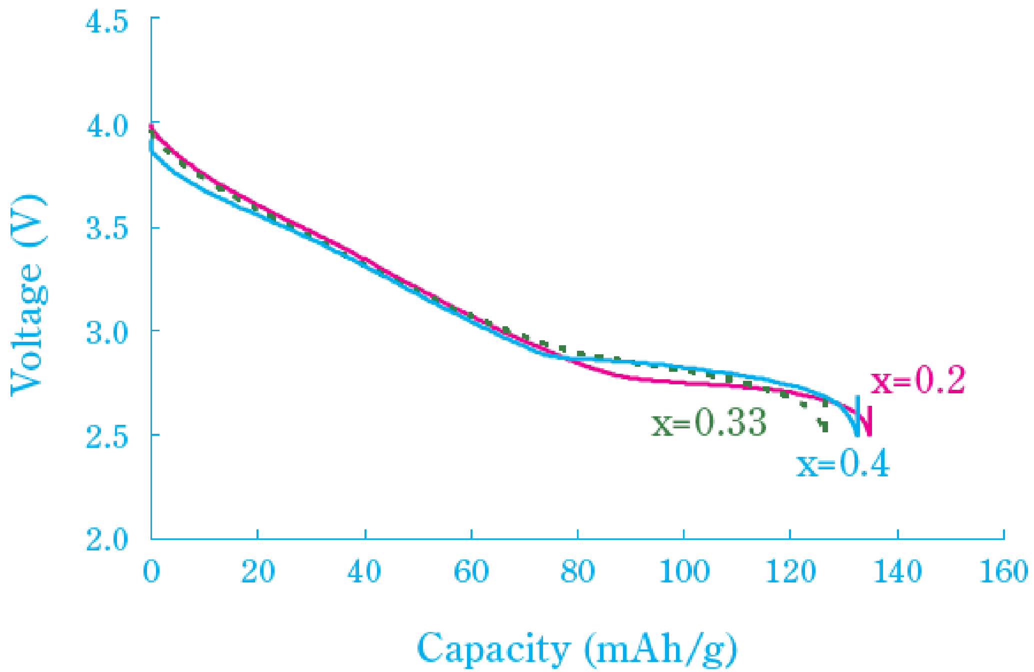
Hard carbon
PBA

A. Bauer et al. Adv. Energy Mater. (2018) 8, 1702869

P2/O3 layered oxides: SoA

- **SoA:**
  - Sumitomo Chemicals Co. Ltd.
    - O3-$NaFe_xMn_{1/2-x/2}O_2$ (x = 0.2, 0.33 and 0.4)
    - Electrolyte: 1M $NaPF_6$ in PC
    - **1st discharge capacity of 135-140 mAh g^{-1}**

	theoretical capacity [mAh/g]	1st charge capacity [mAh/g]	1st discharge capacity [mAh/g]
$Na_{0.7}MnO_2$	182.09	67.0	167.3
$NaFeO_2$	241.82	103.6	60.8
$Na_{0.6}CoO_2$	153.55	84.6	63.1
$NaFe_{0.2}Mn_{0.4}Ni_{0.4}O_2$	240.13	151.4	134.8
$NaFe_{0.33}Mn_{0.33}Ni_{0.33}O_2$	240.54	153.1	126.6
$NaFe_{0.4}Mn_{0.3}Ni_{0.3}O_2$	240.55	157.4	132.5



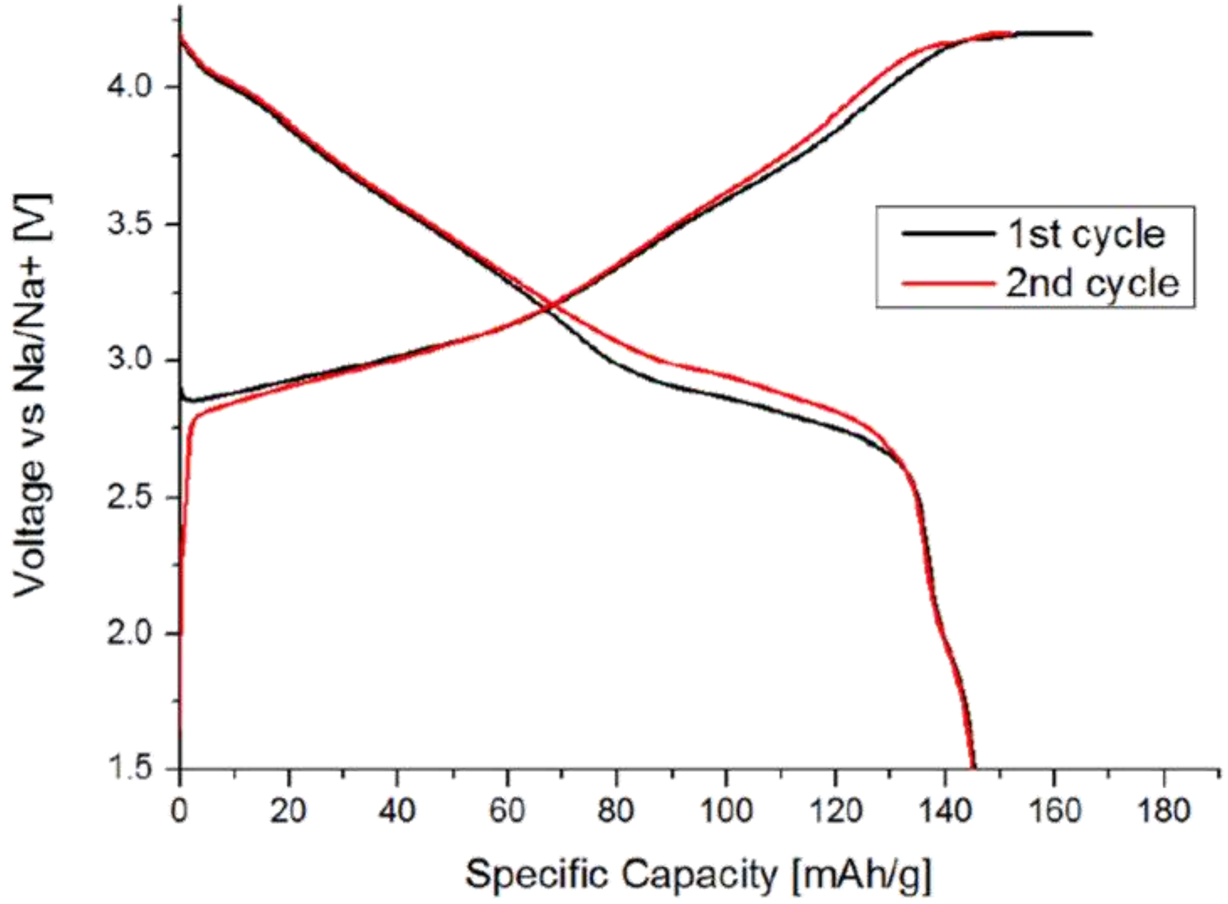
Hard carbon
O3- Mn/Fe/Ni layered oxide

S. Kuze, et al. *R&D Report "SUMITOMO KAGAKU"* (2013)

P2/O3 layered oxides: SoA

SHARP
SHARP LABORATORIES OF EUROPE

- **SoA:**
  - Sharp Laboratories of Europe
    - O3-$NaNiFe_{1/6}Mn_{1/3}Mg_{1/12}Sn_{1/12}O_2$
    - Electrode formulation: 89:5:6 (AM:CB:PVdF)
    - Electrolyte: 1M $NaPF_6$ in EC:DEC (1:1)
    - **Reversible capacities of 147 mAh g^{-1}**
    - 1^{st} loss capacity of 6%



Hard carbon
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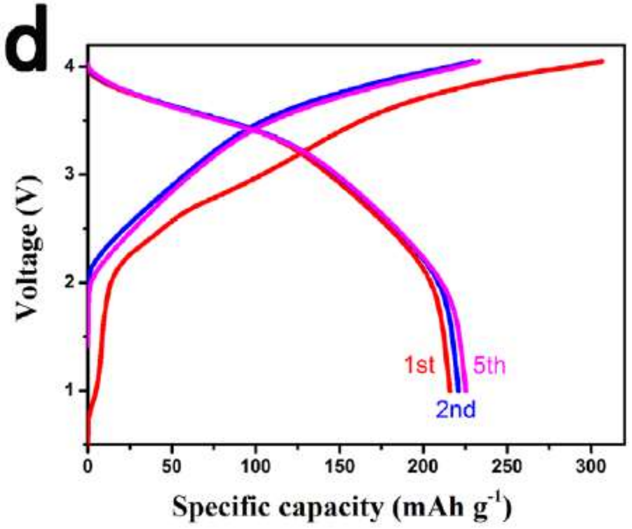
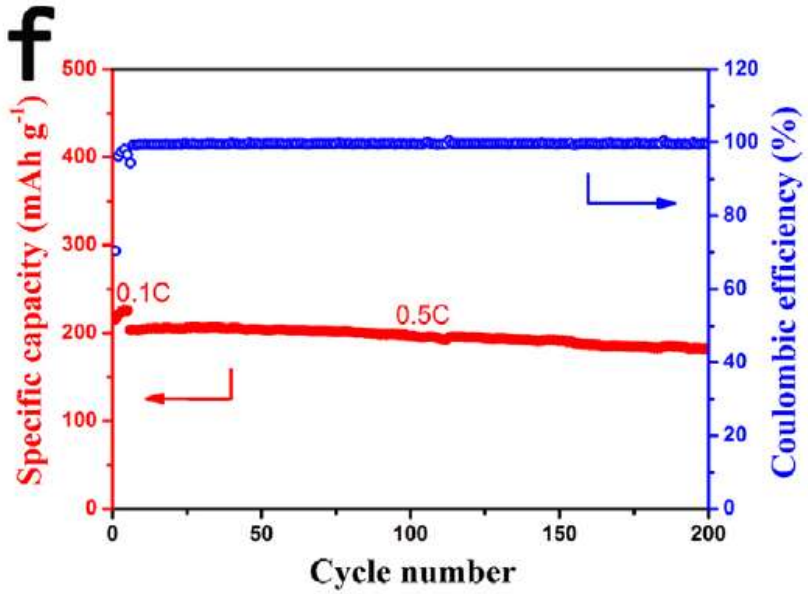
K. Smith, et al. ECS Trans. (2017) 75, 13.

P2/O3 layered oxides: SoA

- **SoA:**
  - HiNa Battery Technology Co.
    - O3-$Na_{0.9}Cu_{0.22}Fe_{0.30}Mn_{0.48}O_2$
    - Electrolyte: 0.8M $NaPF_6$ in EC:DMC (1:1vol%)
    - **Reversible capacities of 222 mAh g^{-1} at 0.1C**
    - **Good stability: 90% after 200 cycles**



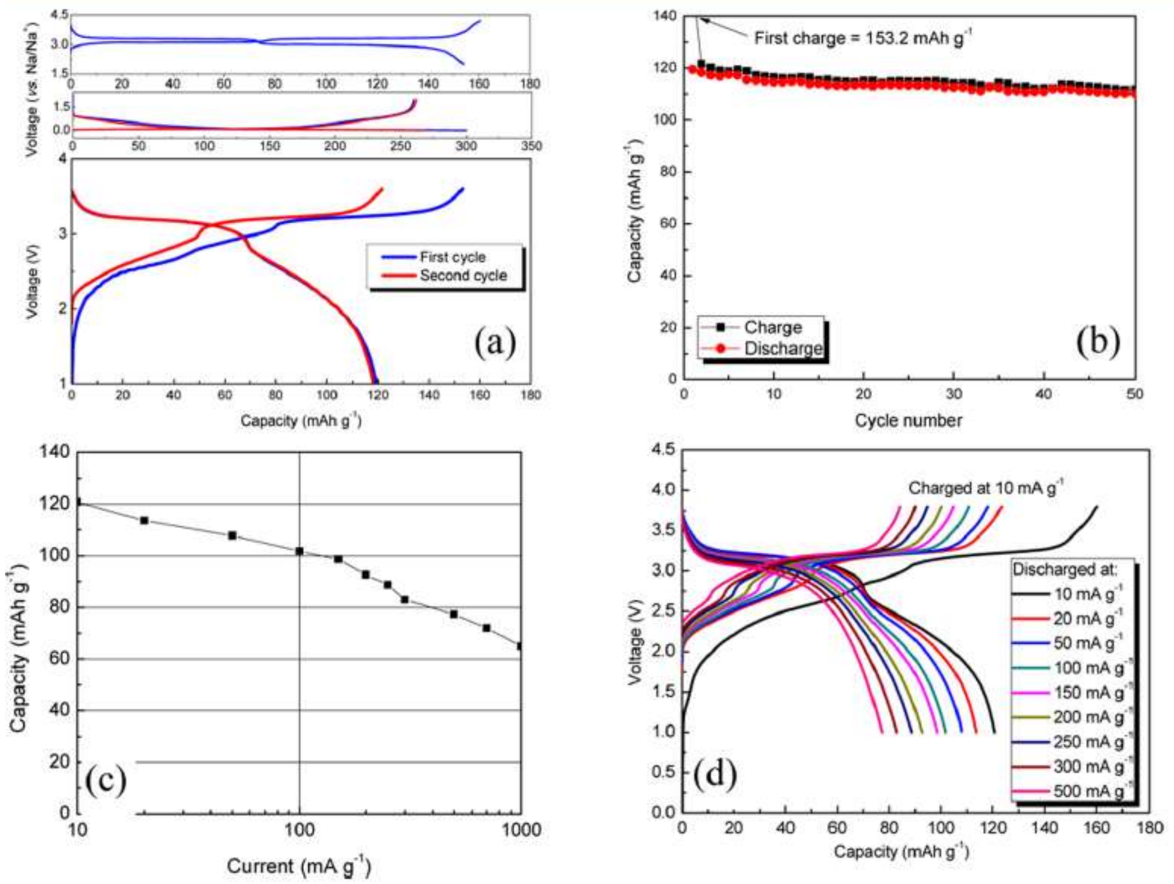


Soft carbon
O3 $Na_{0.9}Cu_{0.22}Fe_{0.30}Mn_{0.48}O_2$

Y. Li et al. Energy Storage Mater. (2016) 5, 191.

Na prototype: Sharp Laboratories of America Inc.

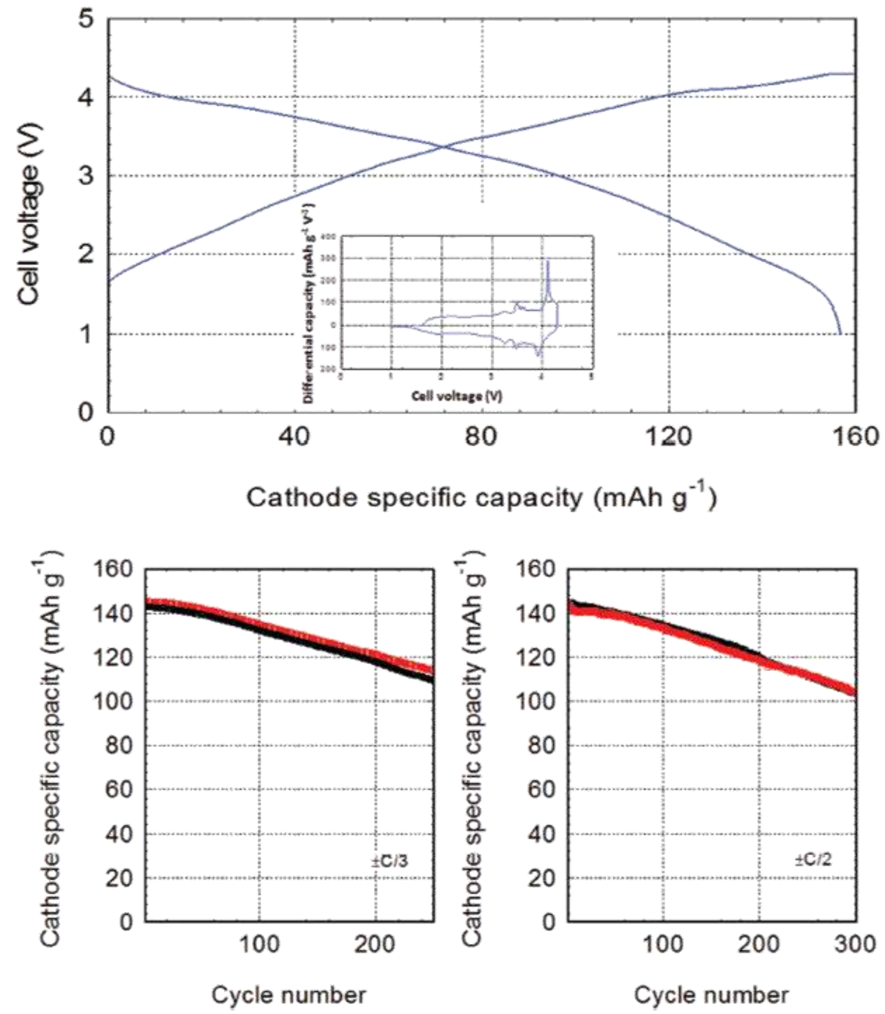
- Anode: **commercial Hard carbon (Kureha)**
  - ICE: 86%
  - Electrode formulation: 95:5 (AM:CMC)
- Cathode: **rhombohedral $Na_{1.92}Fe_2(CN)_6$ (R-FeHCF) Prussian White**
  - Initial delivered a capacity: 160 mA h g^{-1}
  - Average operating voltage: V
  - Electrode formulation: 86:7:7 (AM:KB:PTFE)
- Na-prototype details:
  - Cathode/Anode ratio: 5% excess of anode
  - Electrolyte: 1M $NaPF_6$ in EC:DEC + 5wt% FEC
  - Average full cell voltage: 3 V
  - Initial charge capacity: 153.1 mAh g^{-1}
  - ICE: 78%
  - Capacity retention: 94% after 50 cycles



L. Wang, et al. J. Am. Chem. Soc. 2015, 137, 2548.

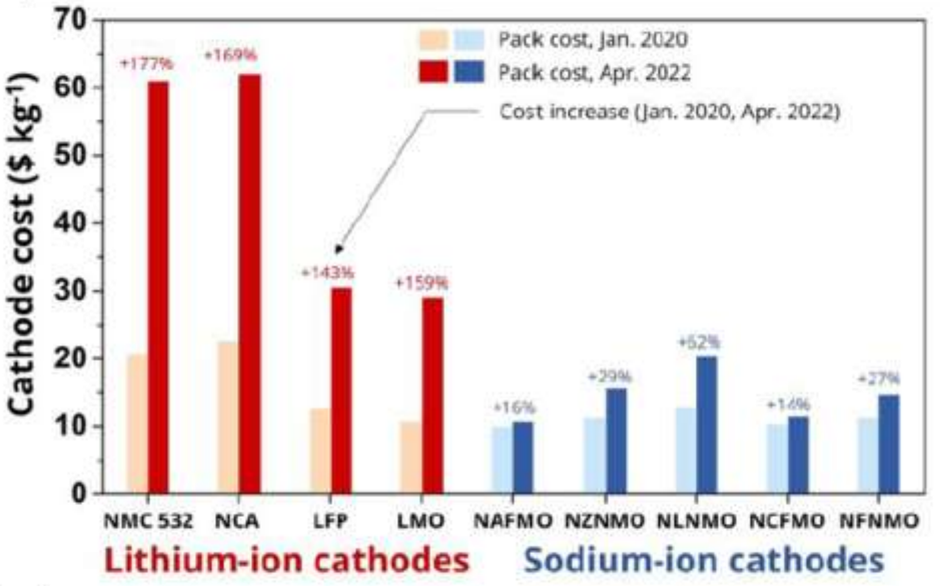
Na prototype: Faradion Ltd.

- Anode: **commercial Hard carbon**
  - Average particle size (d50) : 9 µm
  - SSA: 2 $m^2\ g^{-1}$
  - Delivered capacity: 250 - 300 mA h g^{-1} at low rate, in half-cell
  - Electrode formulation: 88:3:9 (AM:CB:binder)
- Cathode: **O3-$Na_aNi_{(1-x-y-z)}Mn_xMg_yTi_zO_2$**
  - Delivers a capacity: 157 mA h g^{-1}
  - Average operating voltage: 3.2 V
  - Electrode formulation: 89:5:6 (AM:CB:Binder)
- Na-prototype details:
  - Cathode/Anode ratio: 1.5–1.0
  - Electrolyte: 5m $NaPF_6$ in EC:DEC:DMC:PC
  - Cell energy density: 120 W h kg−1 or 230 W h L−1
- Development of NIBs pack for e-bike 400 Wh



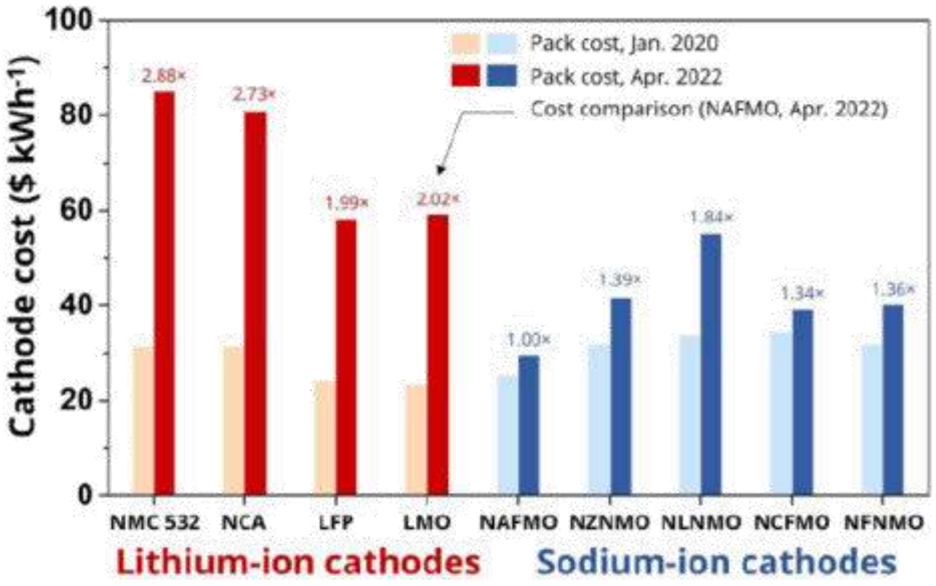
Material cost analysis: Na- vs Li-based

- **Co-free materials lower cost**
- Li-based materials cost increased 143%
- **Na-based materials cost increases 14-16%**



More stable cost for Na-based materials

- **Na cathode cost per kW h^{-1} higher tan Li**
  - Still optimize the performance of NIBs
- Li cost increases → NIBs will be cheaper



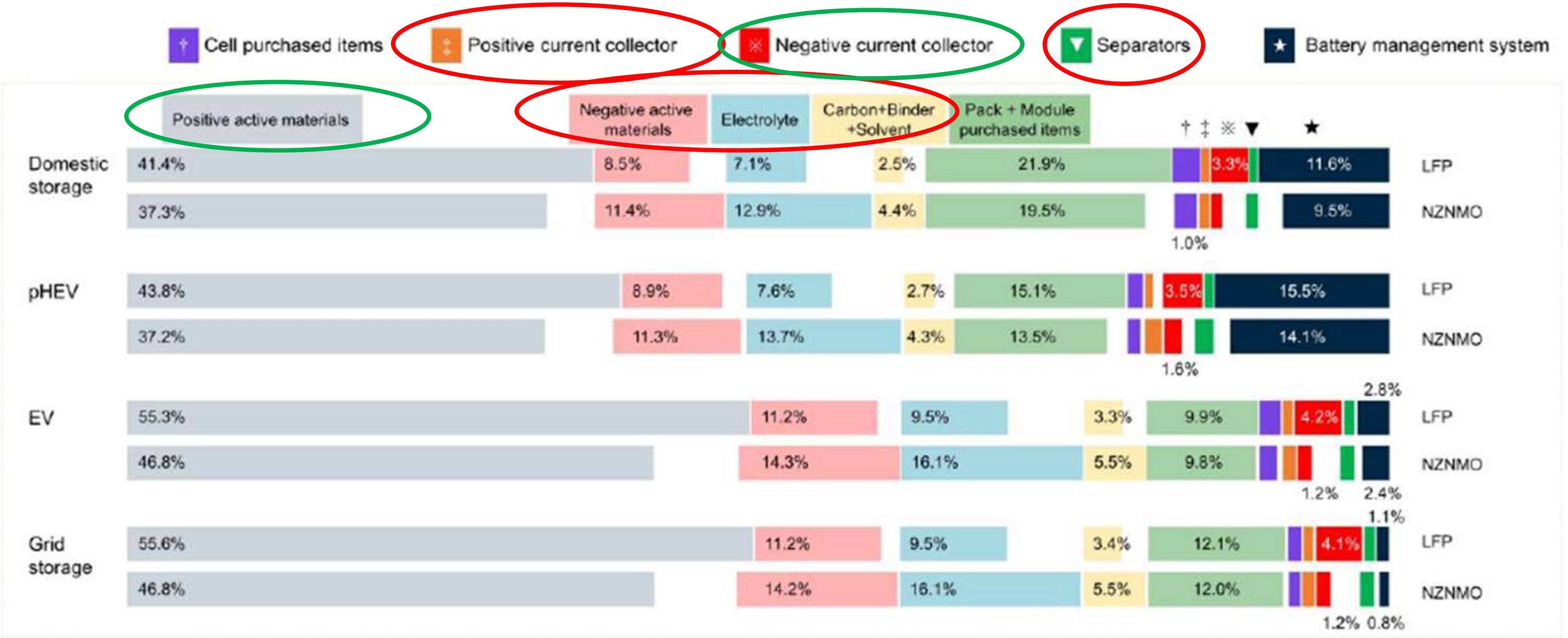
NIBs still should be optimized

Cost of Li-based materials increase → NIBs low-cost EES

Na_xTMO_2 cathodes cost advantage over Li-based

W. Zuo, A. Innocenti, M. Zarrabeitia, D. Bresser, Y. Yang, S. Passerini Account of Chemical Research (submmited – under revision).

Pack compoments cost: LFP- vs NZNMO-based



Cost advantage on positive active materials and negative current collector

LFP: LiFePO4 / graphite
NZNM: Na0.67Zn0.06Ni0.26Mn0.67O2 / hard caron

W. Zuo, A. Innocenti, M. Zarrabeitia, D. Bresser, Y. Yang, S. Passerini Account of Chemical Research (submmited – under revision).

Summary

Optimized SIMBA materials (three anodes: SiCN, SiOC and Hard carbon; and PW cathode) overcome several electrochemical properties the materials used for Na prototypes

Lower cost of Na-based materials (the cost differences with respect to Li-ones is increasing every year)

The electrochemical performance of Na-based materials still should be improved to reduce the NIBs cost, in terms of $/kW h

SIMBA is focused on 2nd generation on NIBs, using aqueous processing binder (easier to recycle) and novel and safe solid-state electrolyte

Thank you!

SIMBA
SODIUM-ION AND SODIUM METAL BATTERIES

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JM Johnson Matthey
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Elkem

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