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Innovation in Energy Storage

A materials chemist's perspective

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Oxford Energy Day
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What's driving energy storage innovation?

Consumer electronics

More compact, longer lasting

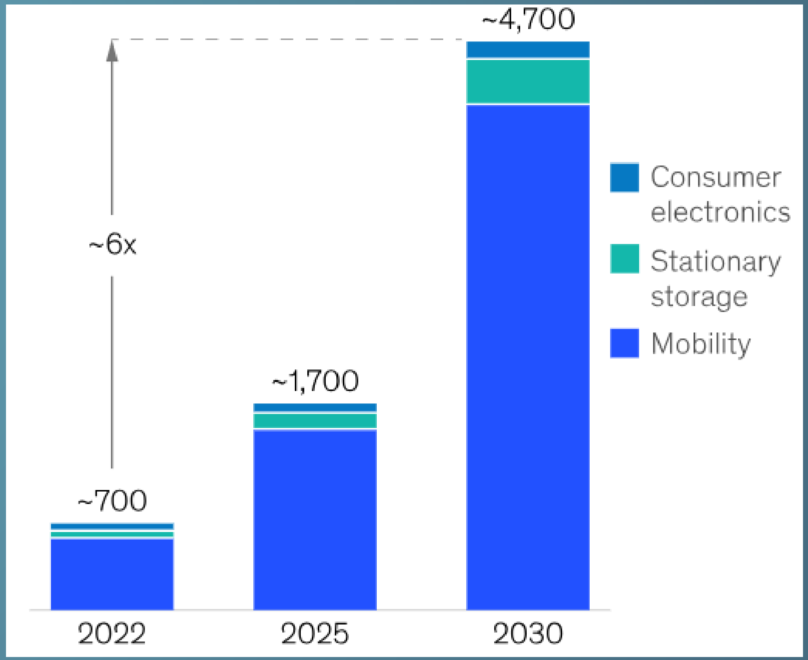
Stationary storage

Low cost, super reliable

Mobility

Low cost, higher energy density, long lifetime

Global Li-ion cell demand (GWh)



McKinsey & Company *Battery 2030: Resilient, sustainable, and circular* (Jan 2023)

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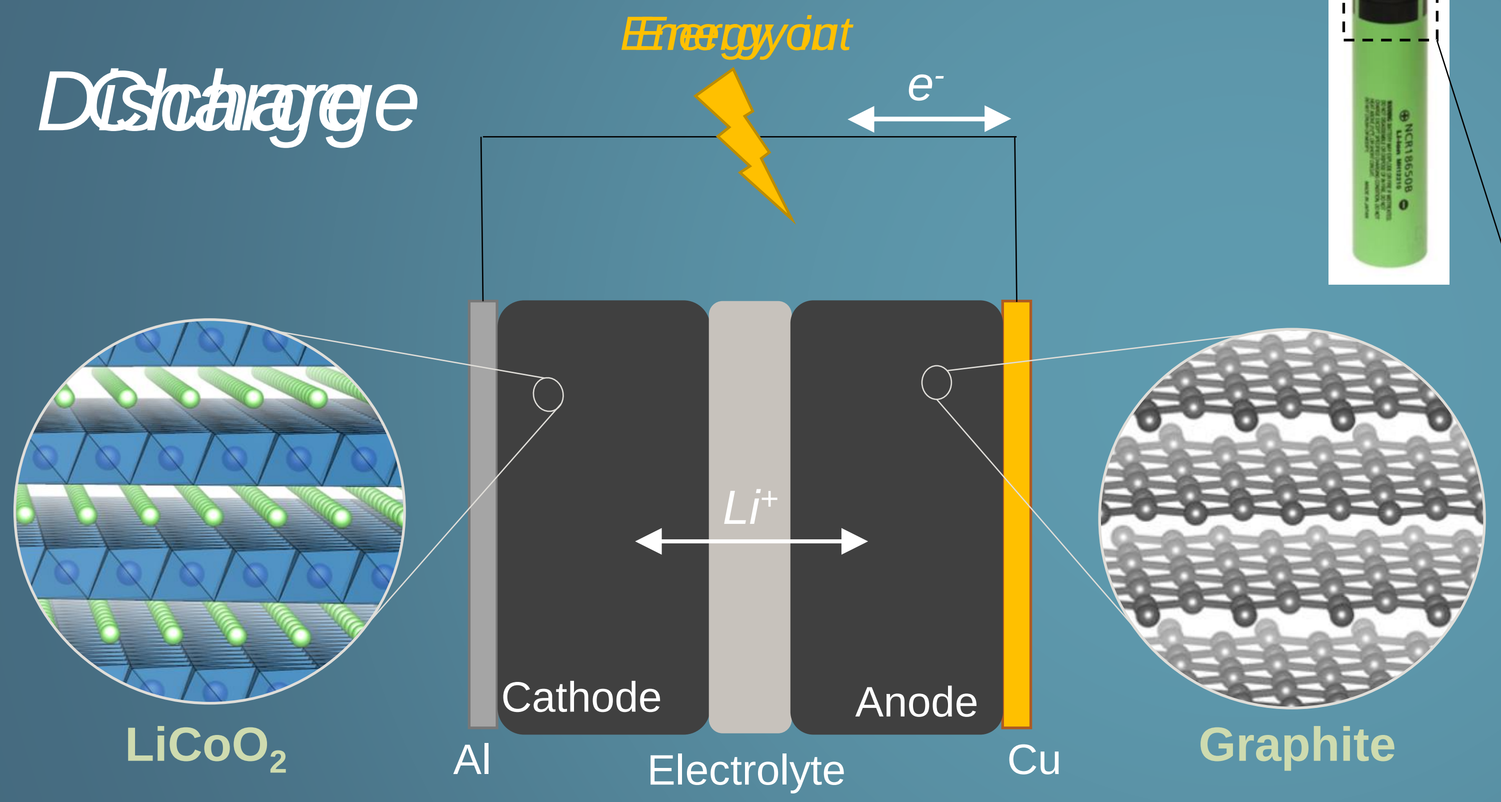
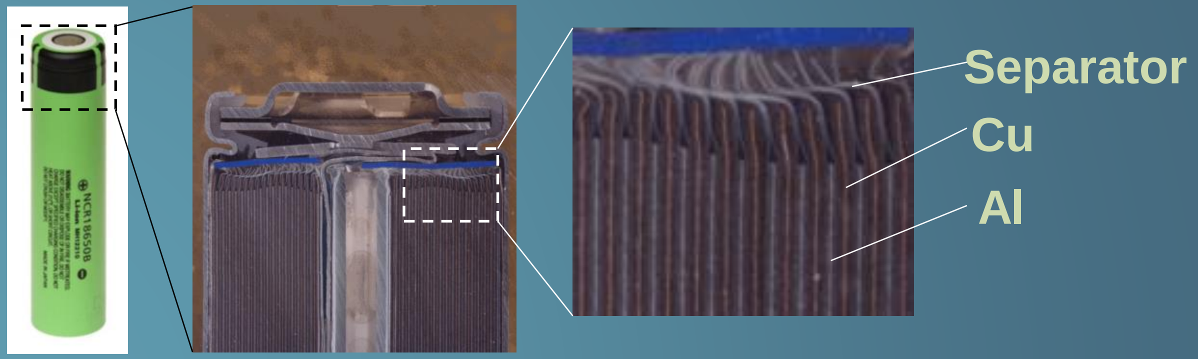
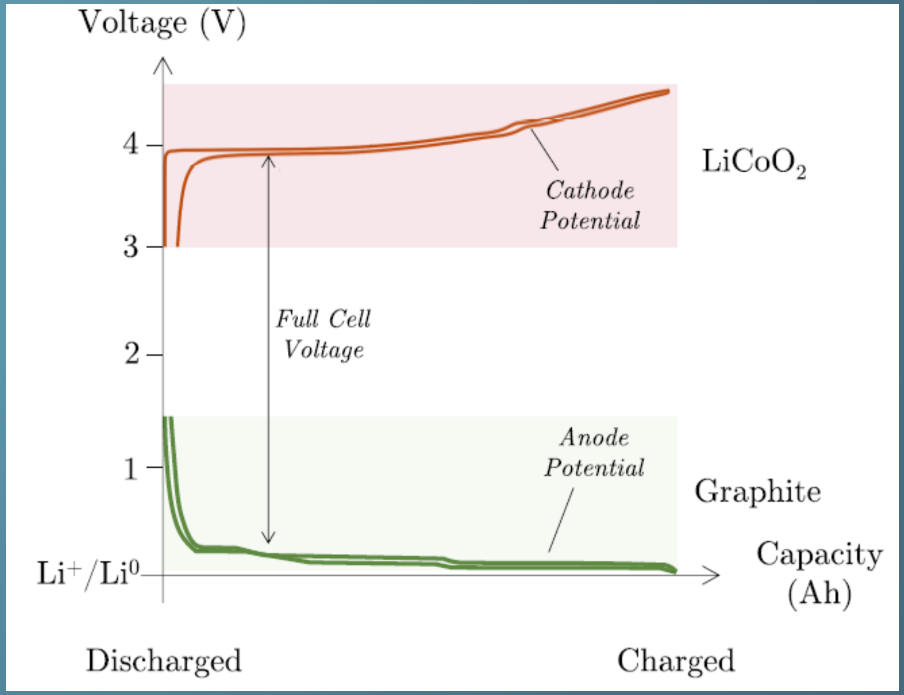
Key automotive drivers of innovation

Barrier to consumer	Technology barrier
Too expensive	• **Cost** of battery is ~50% of car • Mainly due to high raw material cost • Reduce reliance on Li, Ni, Co
Range anxiety	• **Energy density** of battery needs improving • Increase battery capacity and voltage • New battery materials
Long charging times	• **Power density** of battery needs improving • Faster ion diffusion • New battery materials

How to improve Li-ion



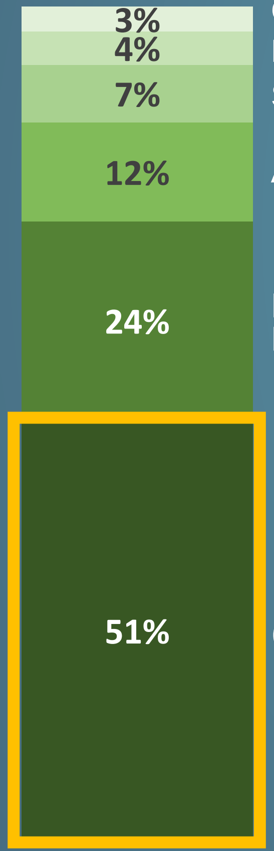




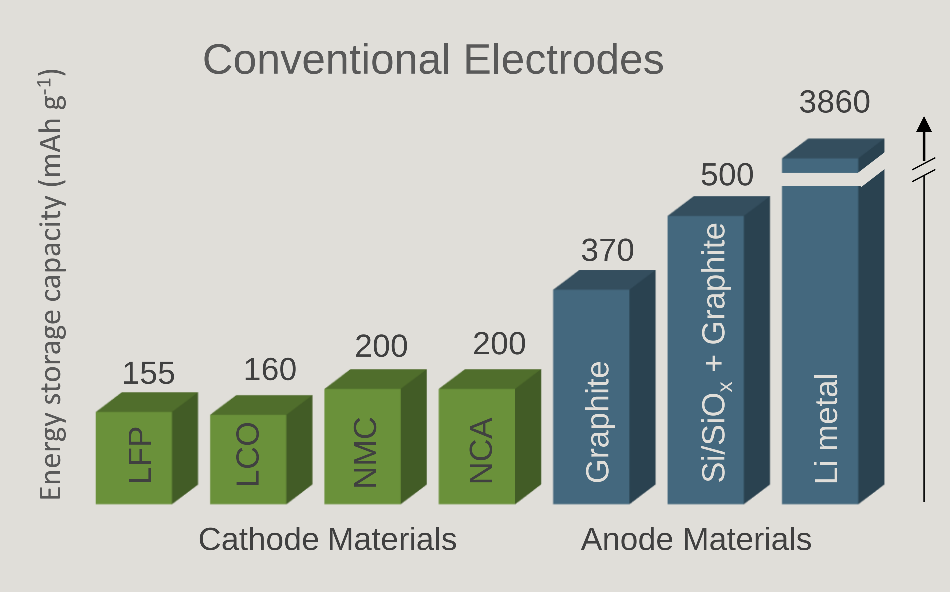
Energy density (Wh kg^{-1}) = Voltage (V) x Capacity (Ah kg^{-1})

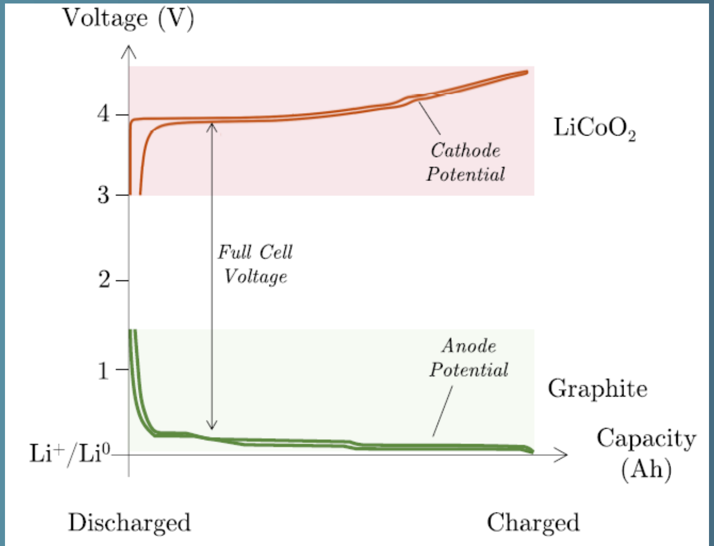
Cathode is a key limitation

Breakdown of cell costs



Bloomberg NEF 2021

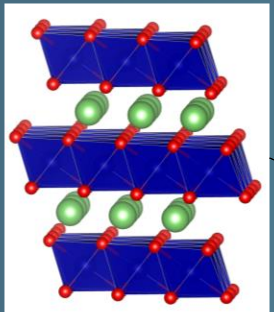




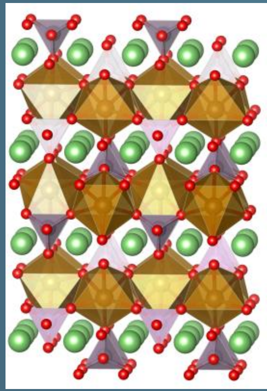
- Lower the **cost** of the cathode material (↓Ni and ↓Co)
- Increase the **voltage** and **capacity** of the cathode

Innovation in Li-ion cathodes

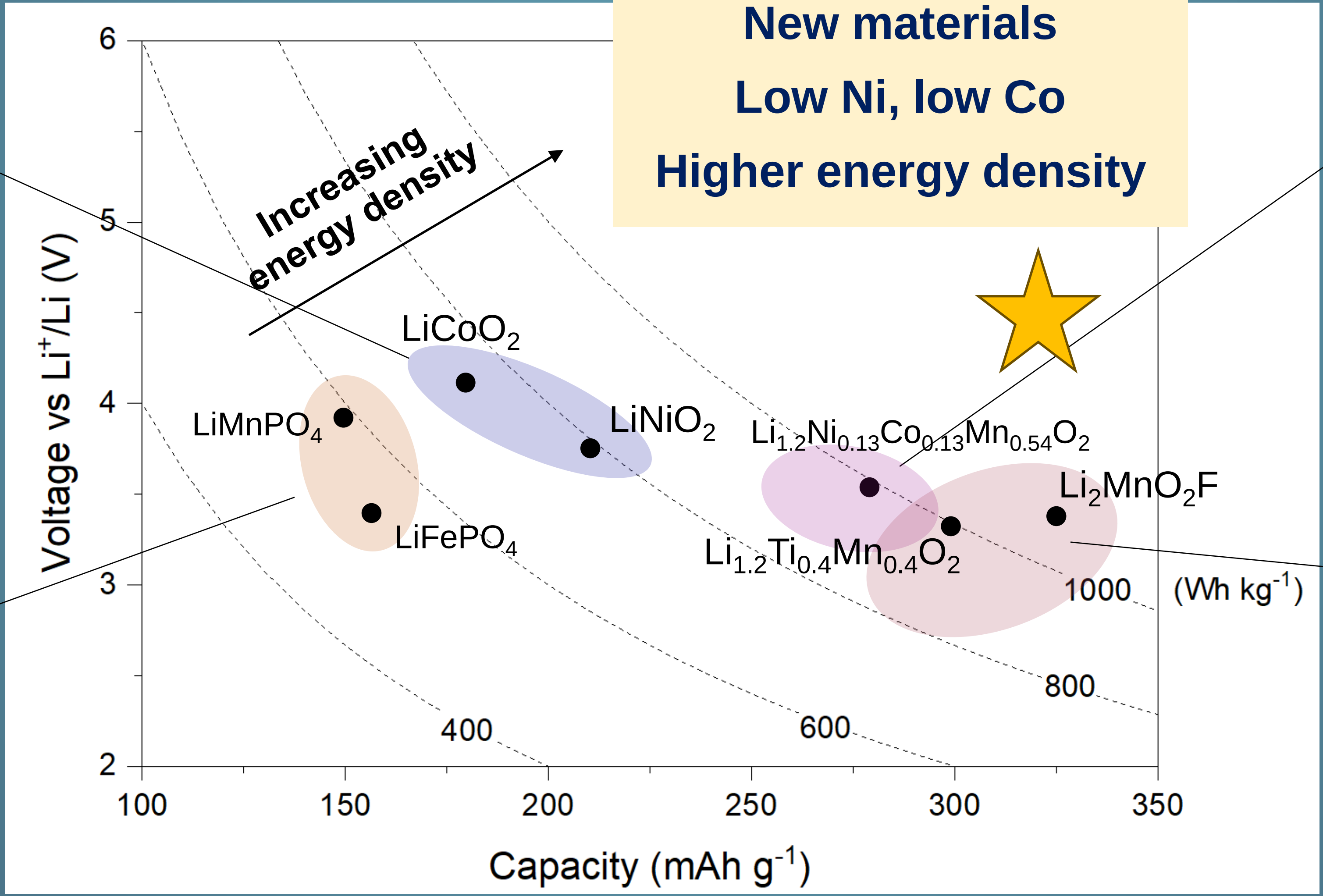
Conventional



Layered



Phosphates

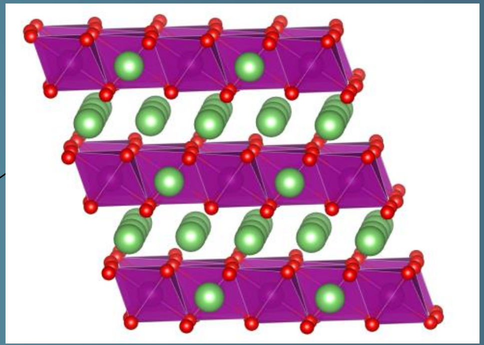


New materials

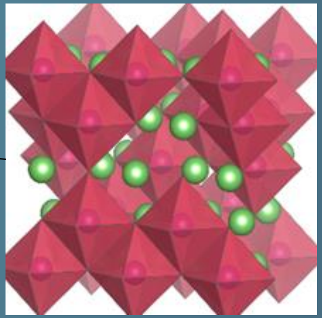
Low Ni, low Co

Higher energy density

Next generation

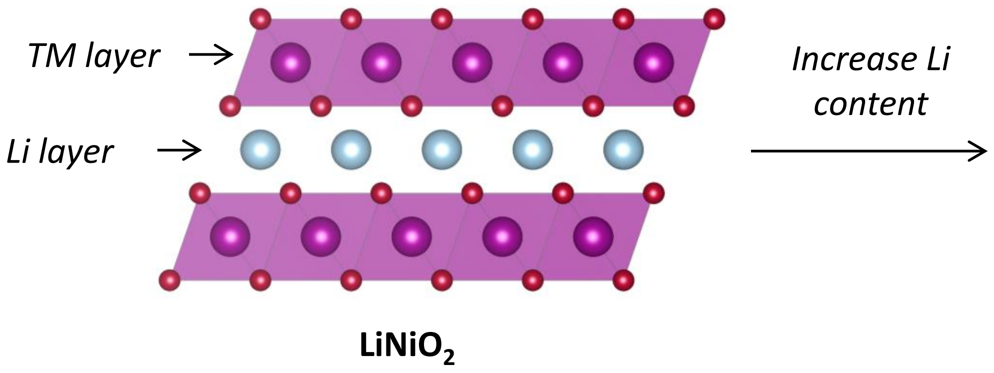


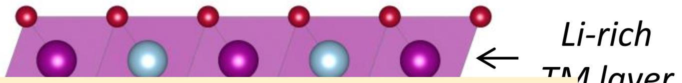
Li-rich



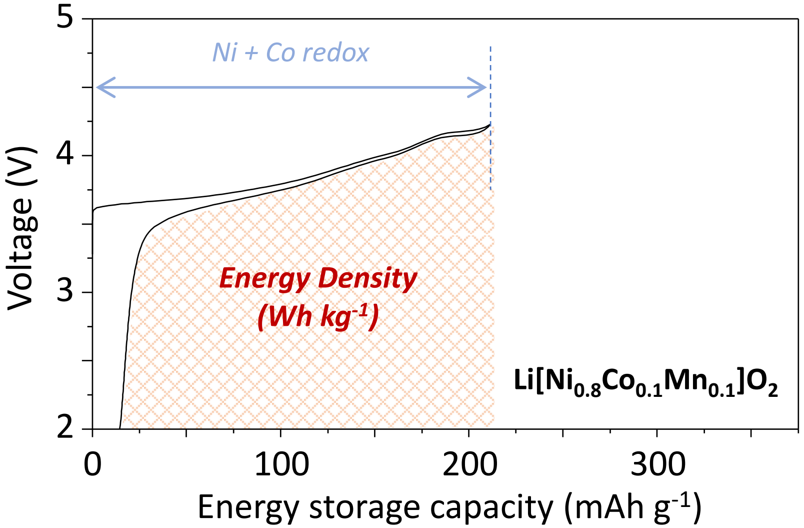
Disordered rocksalt

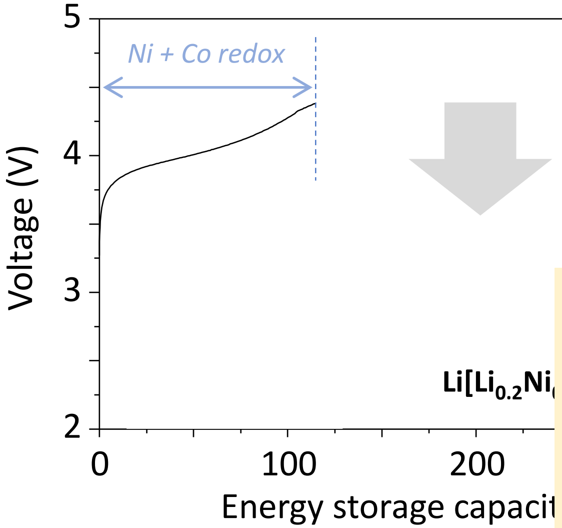
Innovation in Li-ion cathodes





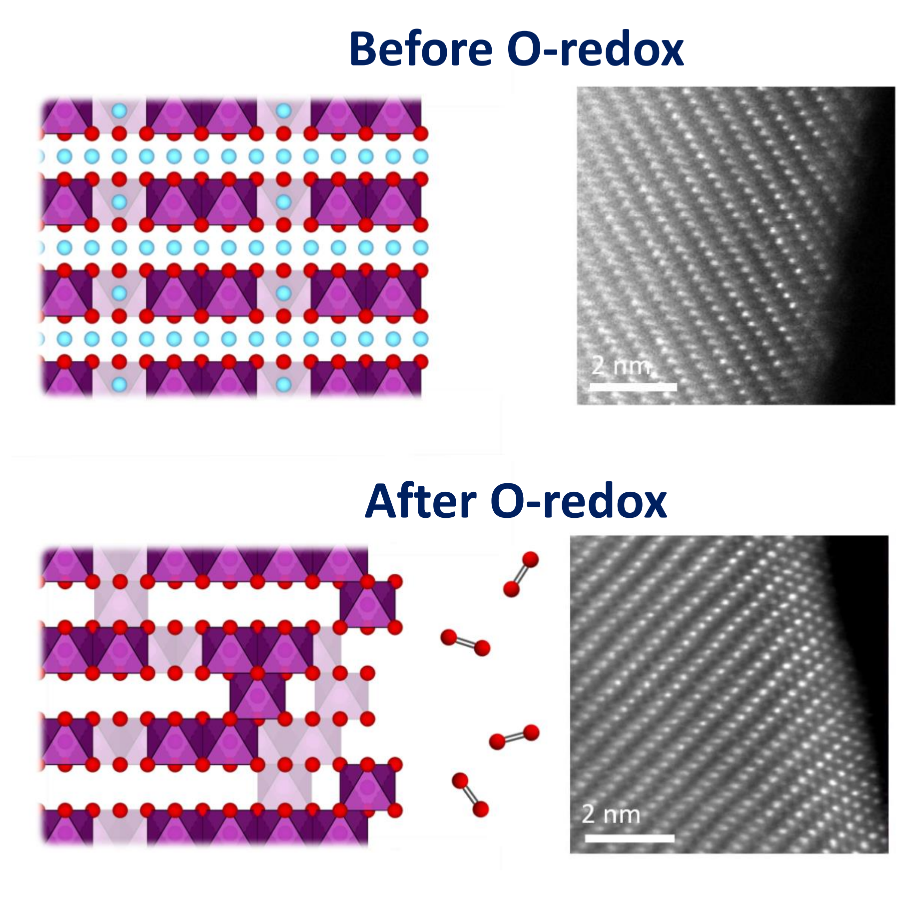
Oxygen-redox could lead to much higher energy density cathodes





Voltage irreversibility needs understanding

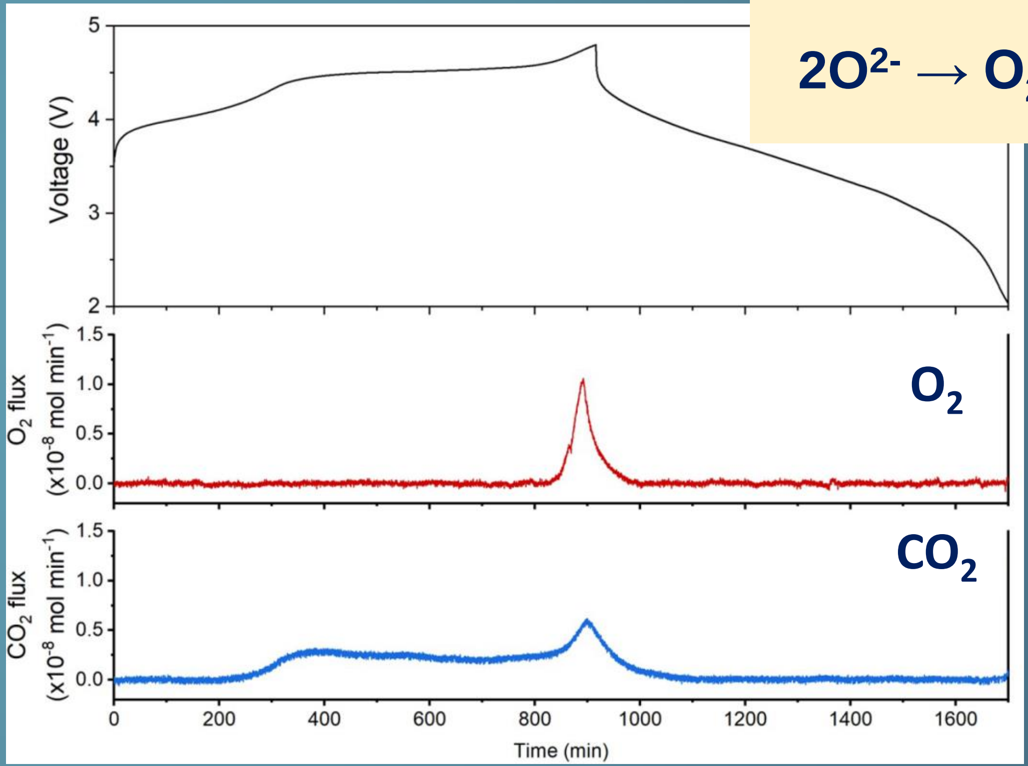
Innovation in Li-ion cathodes



Cathode Particle **Surface**

Operando mass spectrometry

$2O^{2-} \rightarrow O_2 + 4e^-$



Surface oxygen-loss only accounts for 25% of the capacity

What is the bulk mechanism of oxygen redox?

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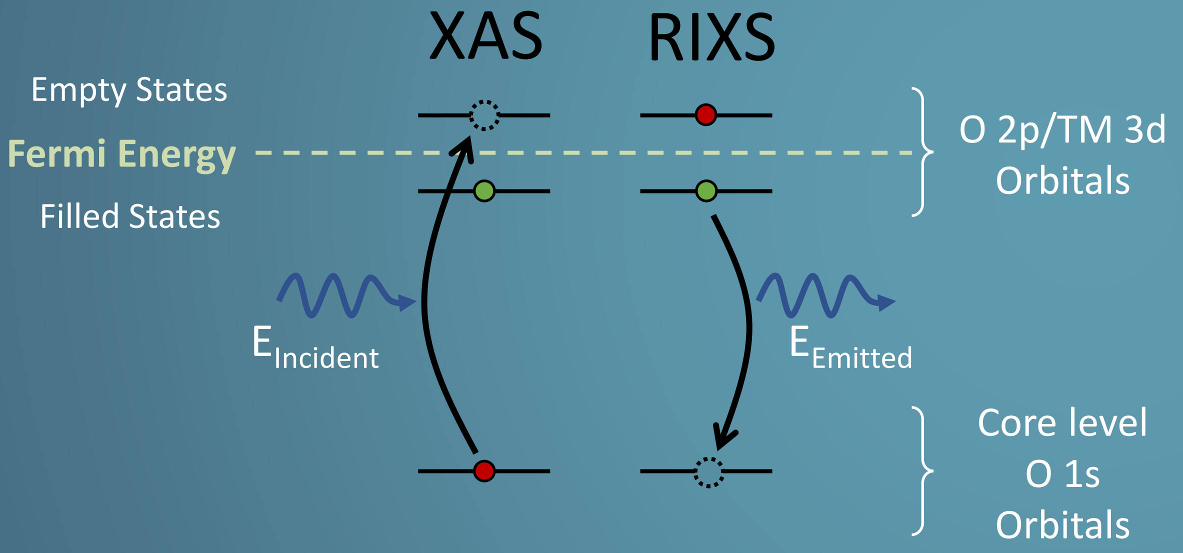
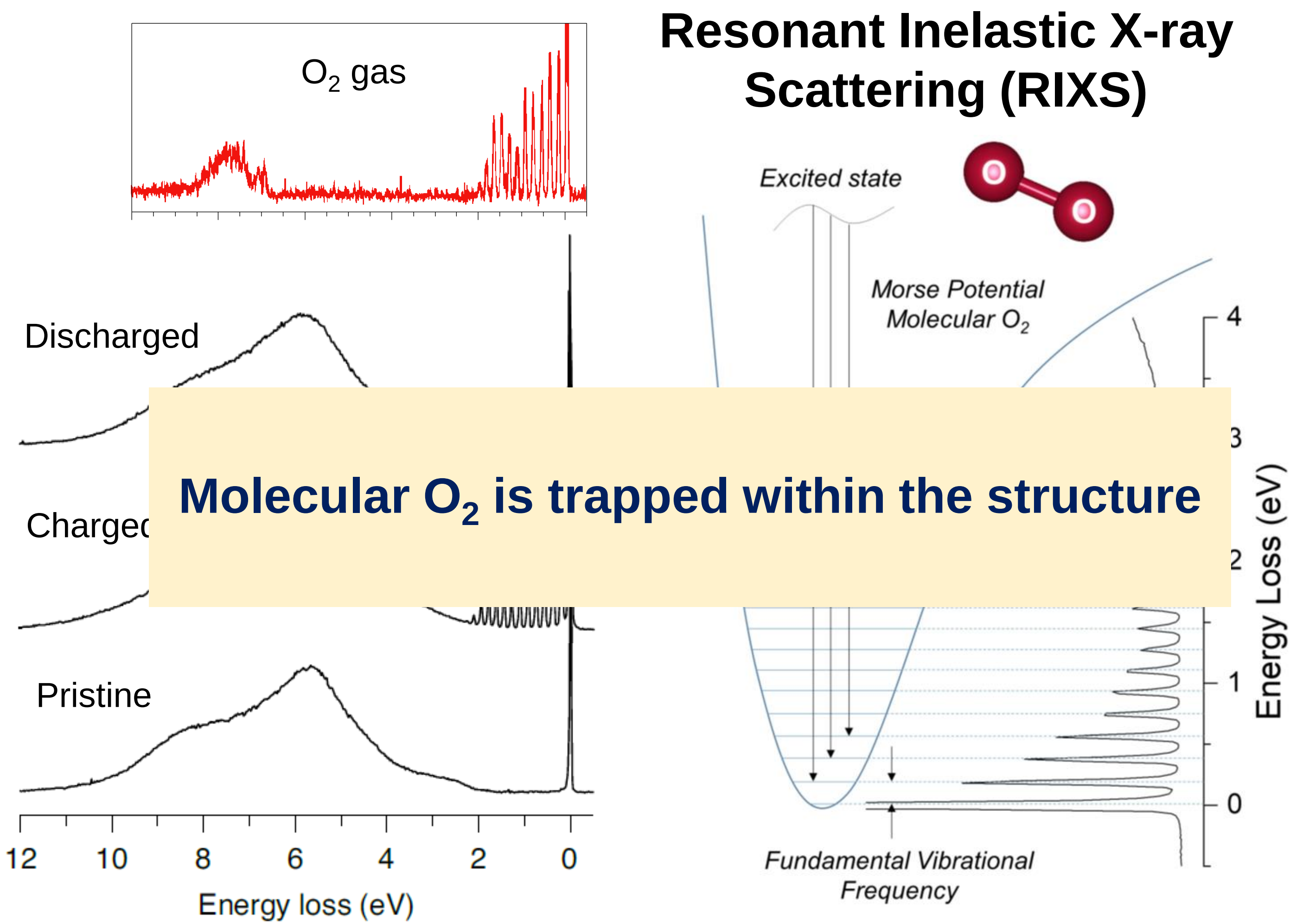
Innovation in Li-ion cathodes

Resonant Inelastic X-ray Scattering (RIXS)



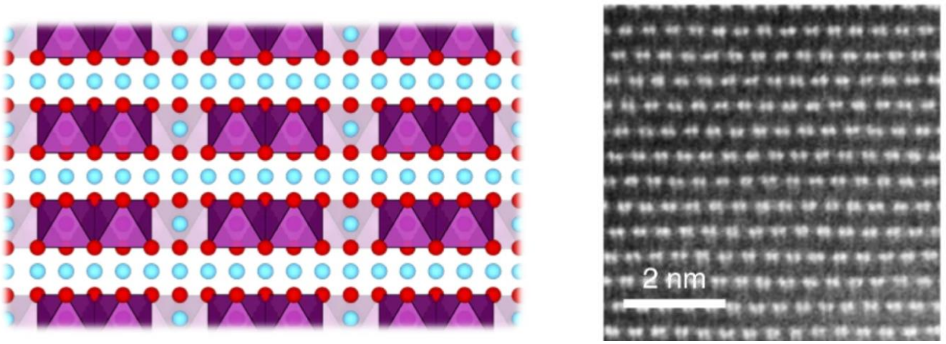
Probing the O valence states with RIXS at the O K-edge

Innovation in Li-ion cathodes

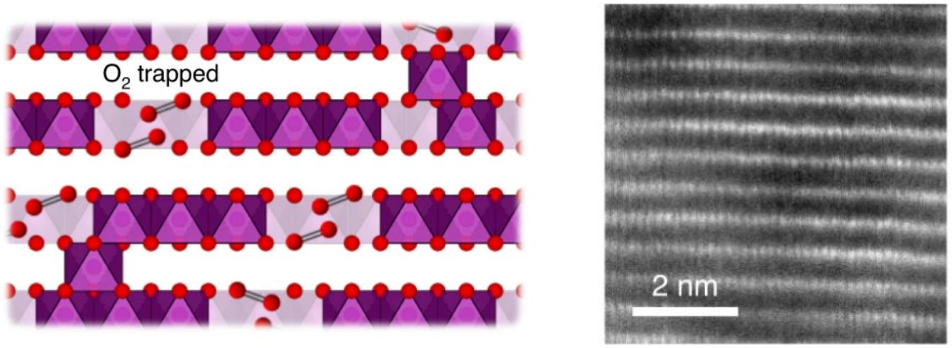


Molecular O_2 is trapped within the structure

Before O-redox



After O-redox

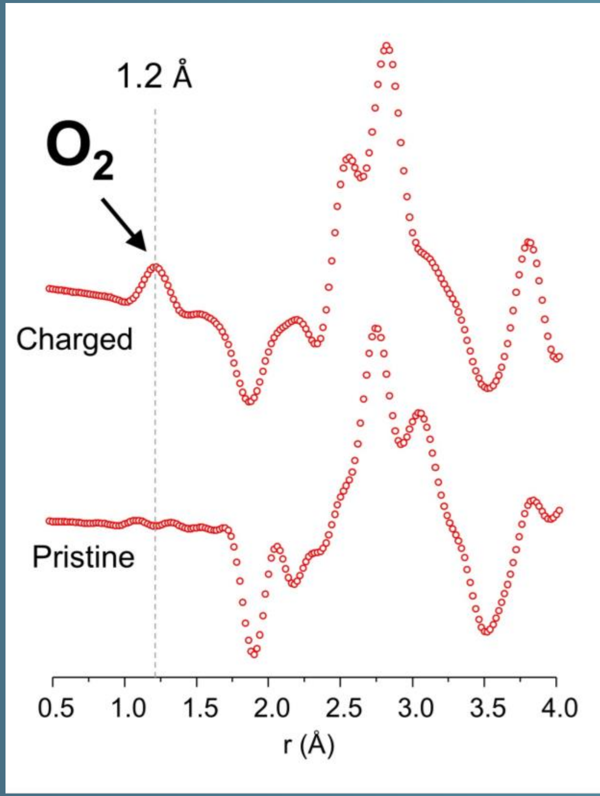


Cathode Particle **Bulk**

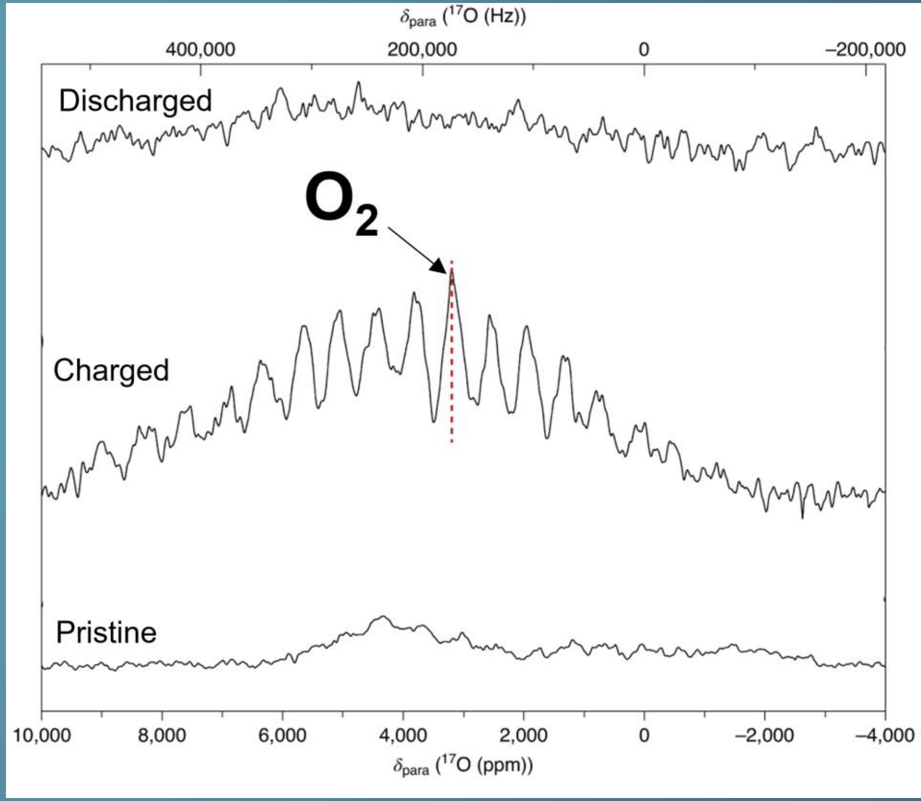
House R.A. et al. *Nature Energy* **5**, 777–785 (2020)

Innovation in Li-ion cathodes

Neutron Total Scattering (PDF)



^{17}O MAS NMR



- Bulk average
- No beam damage
- Quantitative

10-15% of the O in the form of trapped O_2

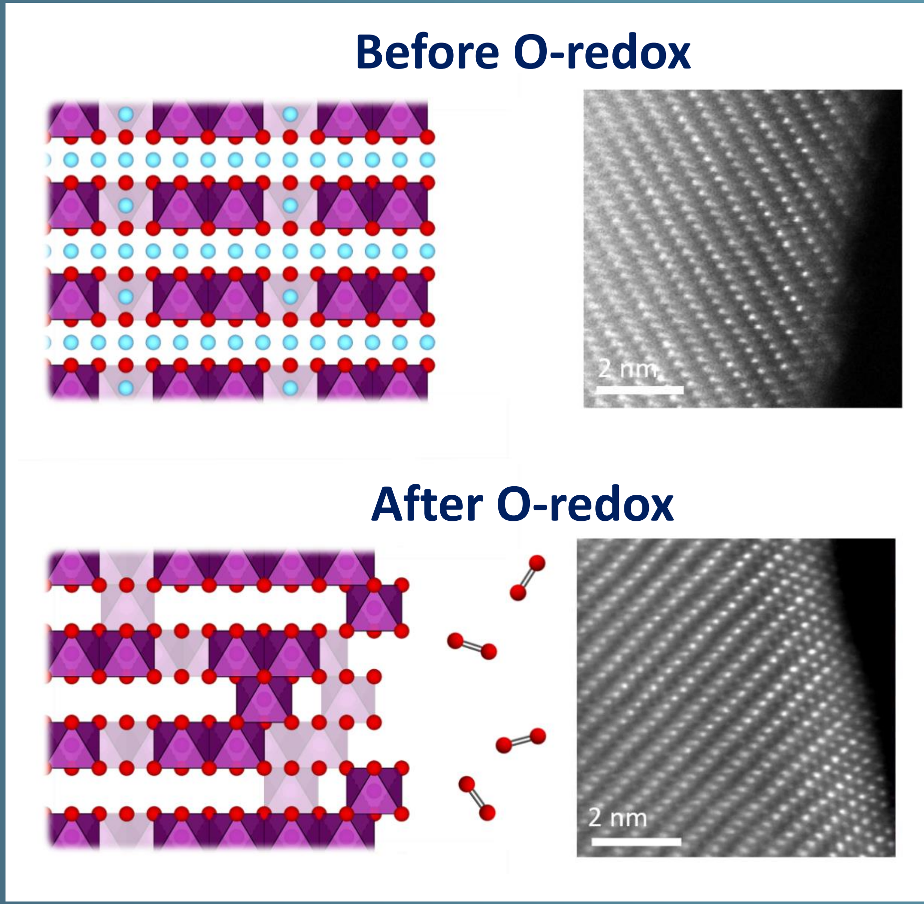
Trapped O_2 corroborated by neutron PDF and ^{17}O NMR

House R.A. et al. *Energy Environ. Sci.*, **15**, 376-383 (2022)

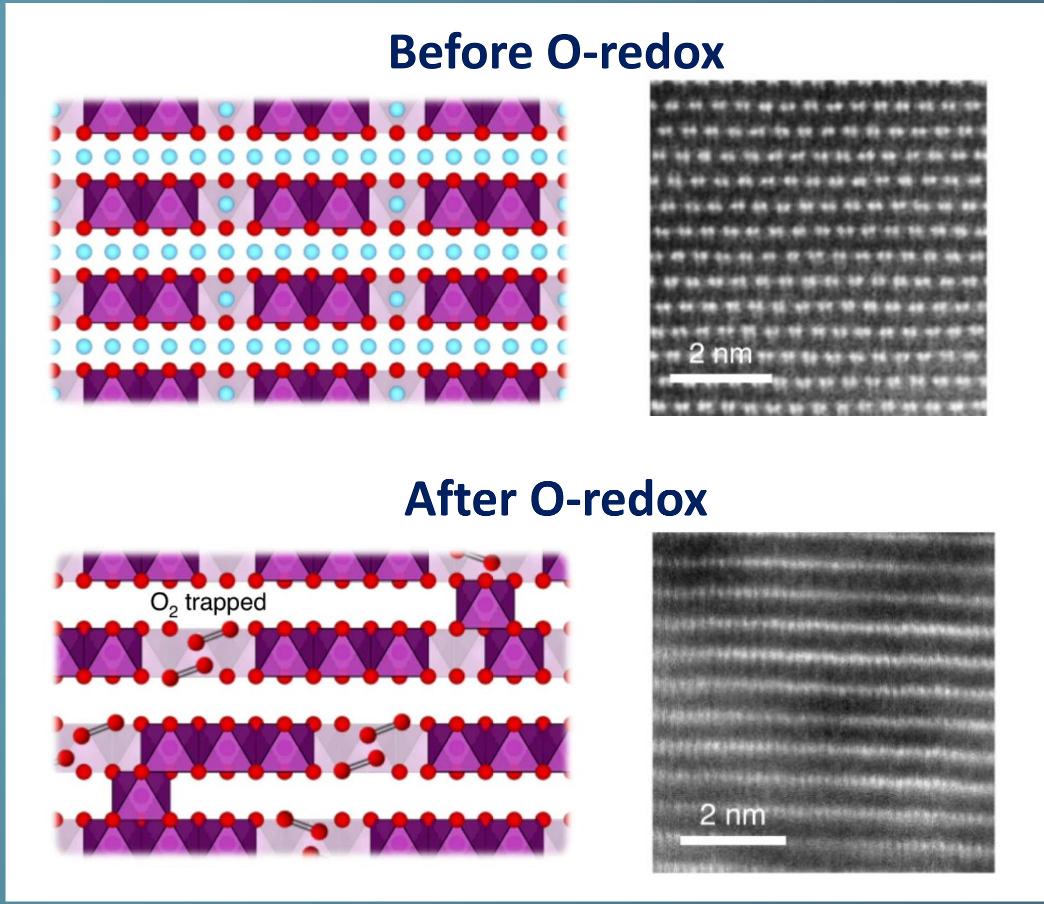
House R.A. et al. *Nature Energy* **5**, 777–785 (2020)

Innovation in Li-ion cathodes

$Li[Li_{0.2}Ni_{0.13}Co_{0.13}Mn_{0.54}]O_2$

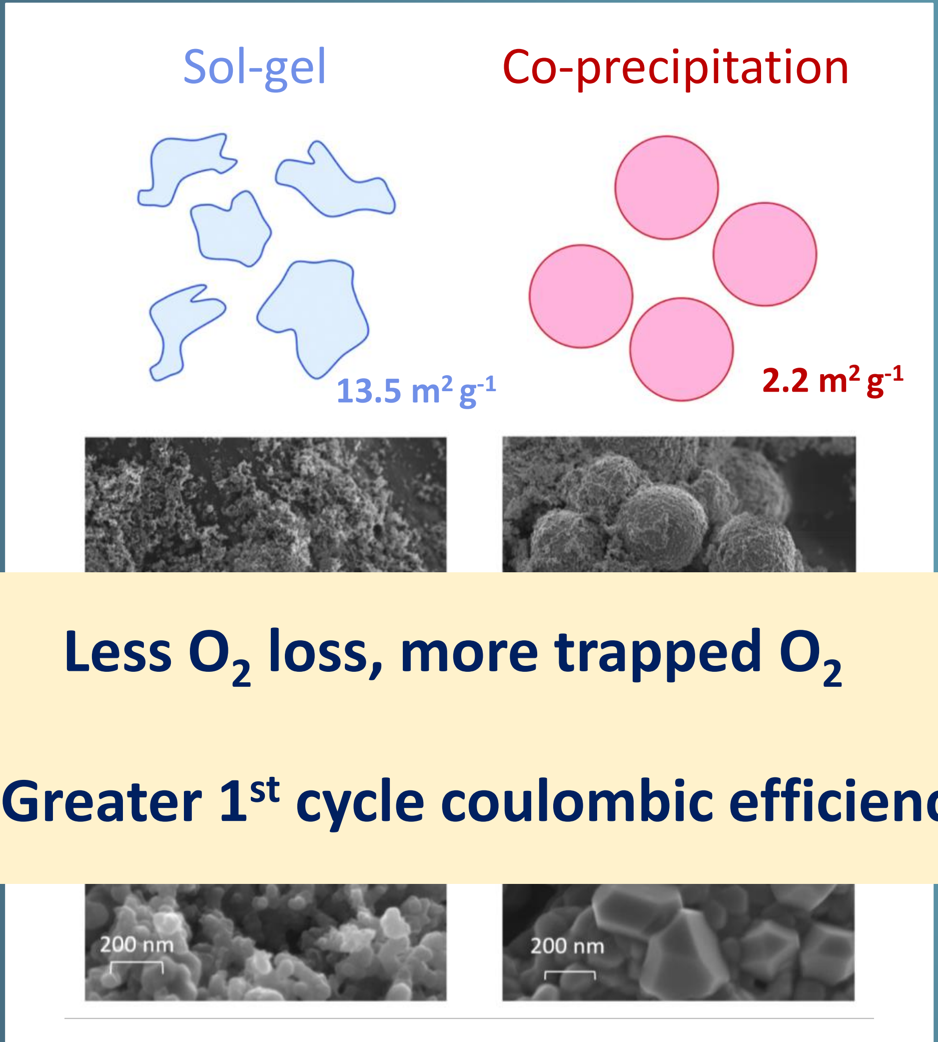


Cathode Particle **Surface**



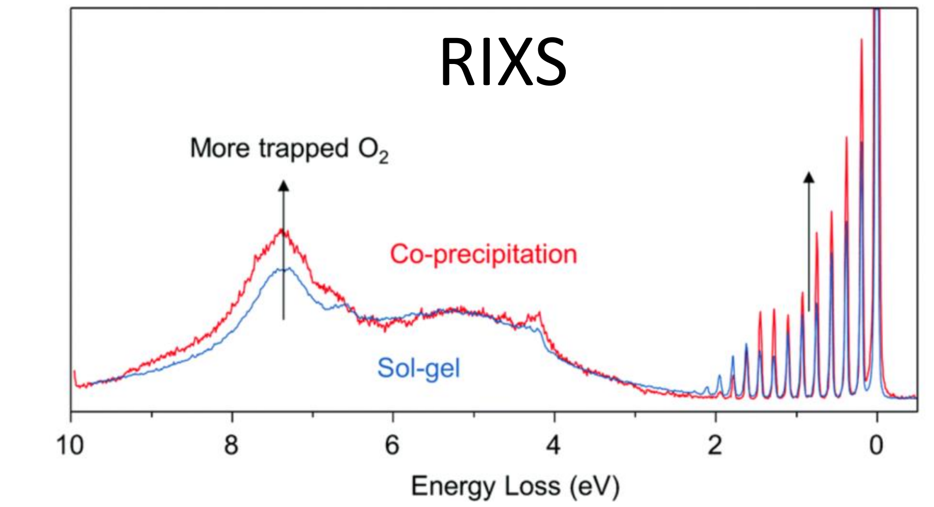
Cathode Particle **Bulk**

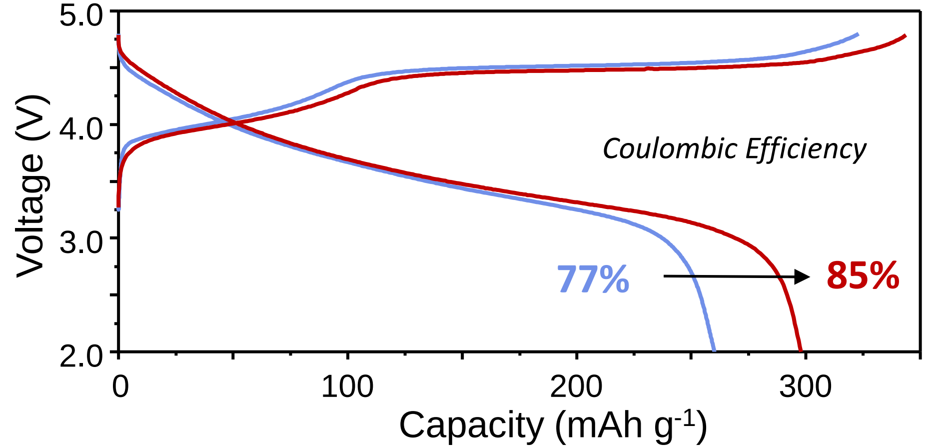
Innovation in Li-ion cathodes



Less O_2 loss, more trapped O_2

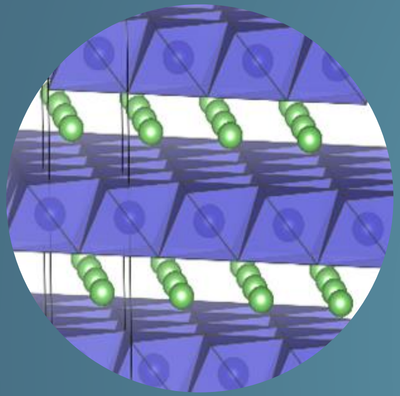
→ Greater 1st cycle coulombic efficiency



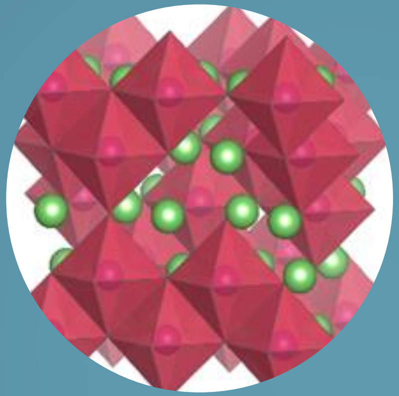


House R.A. et al. *Energy Environ. Sci.*, **15**, 376-383 (2022)

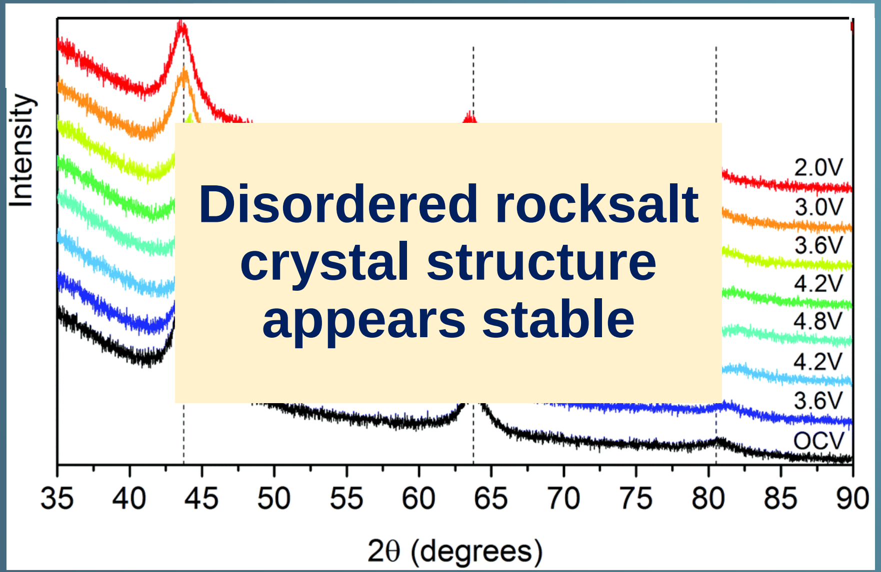
Innovation in Li-ion cathodes



Ordered



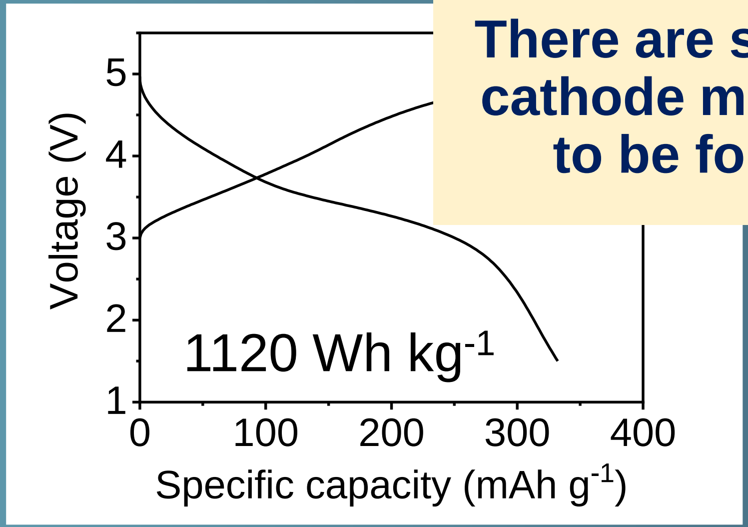
Disordered



Disordered rocksalt crystal structure appears stable

Discharge

Charge



There are still new cathode materials to be found!

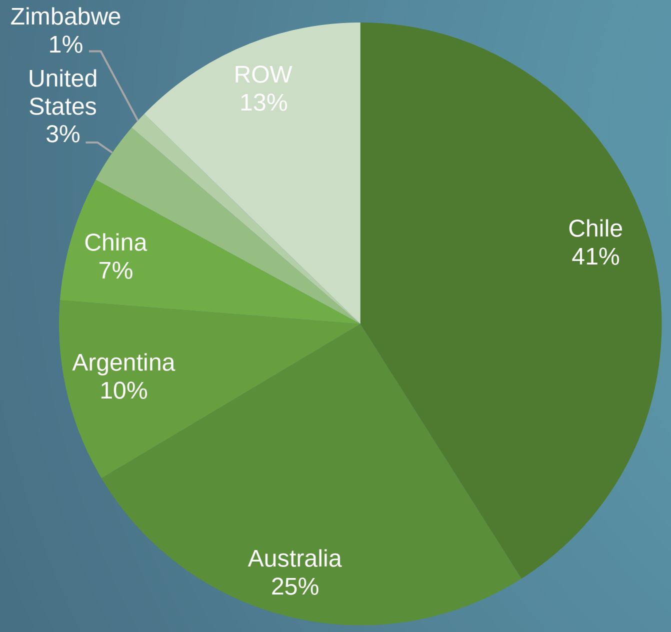
Li_2MnO_2F

Li_2VO_2F	$Li_{1.2}Mn_{0.4}Ti_{0.4}O_2$
Li_2NiO_2F	$Li_{1.3}Mn_{0.4}Nb_{0.3}O_2$
$Li_2Mn_{1/2}Ti_{1/2}O_2F$	$Li_{1.2}Mn_{0.4}Zn_{0.4}O_2$
$Li_2Mn_{2/3}Nb_{1/3}O_2F$	$Li_4Mn_2O_5$

House et al. *Energy & Environ. Sci.* **11**, 926-932 (2018)

Lithium isn't perfect

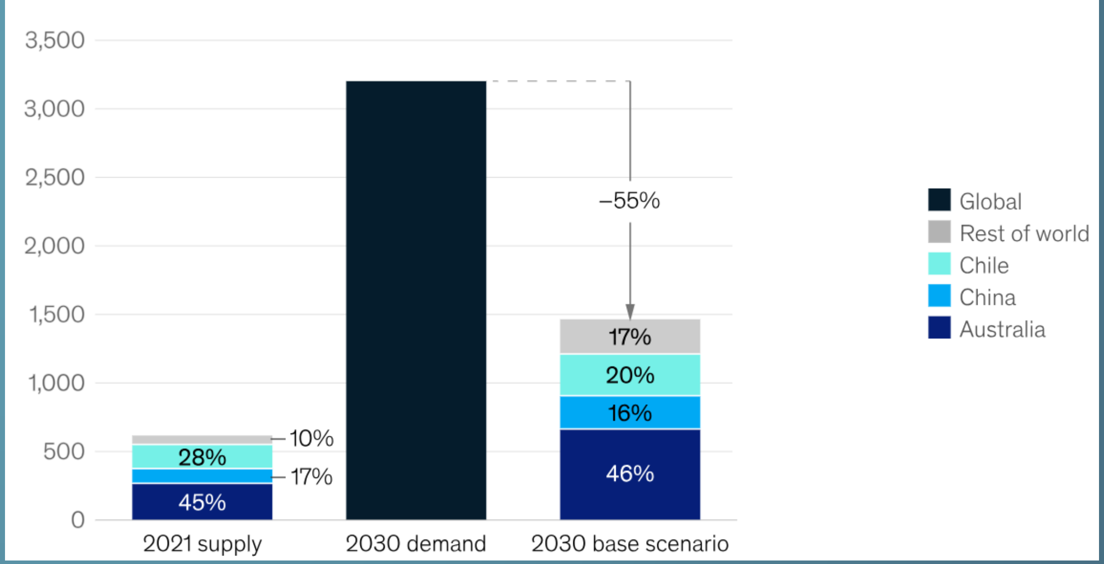
Global mineral reserves of lithium



US Geological Survey 2022

Majority of lithium located in 4 countries

Lithium carbonate global demand vs supply (kilotonnes)



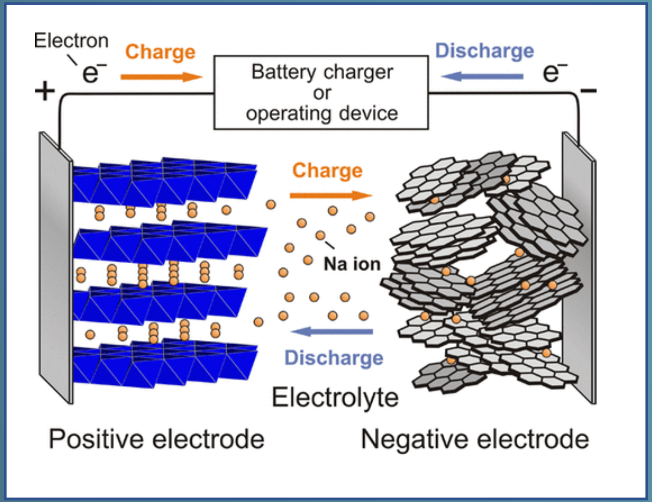
McKinsey & Company *Battery 2030: Resilient, sustainable, and circular* (Jan 2023)

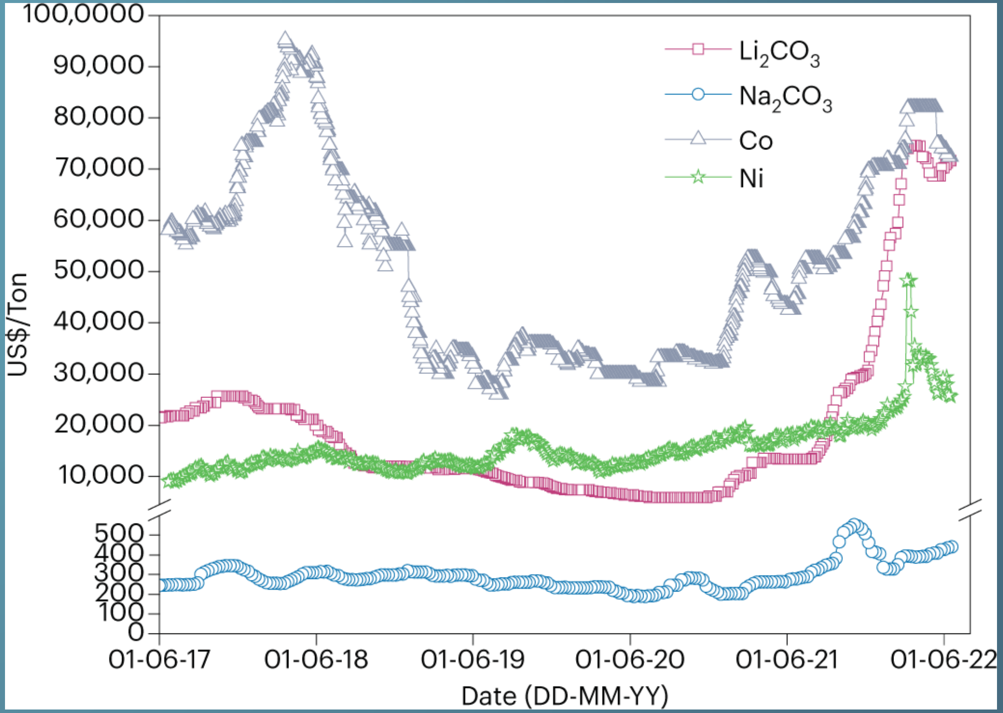
Lithium could be in short supply

Enter… sodium-ion batteries

Naturally occurring soda ash (rocks and brines) → Sodium carbonate → Na-ion batteries

Limestone + salt (solvay process) → Sodium carbonate





Rudola et al. *Nature Energy* **8**, 215–218 (2023)
Data taken from tradingeconomics.com

- Drop-in replacement for Li-ion and Pb-acid
- Same manufacturing methods as Li-ion

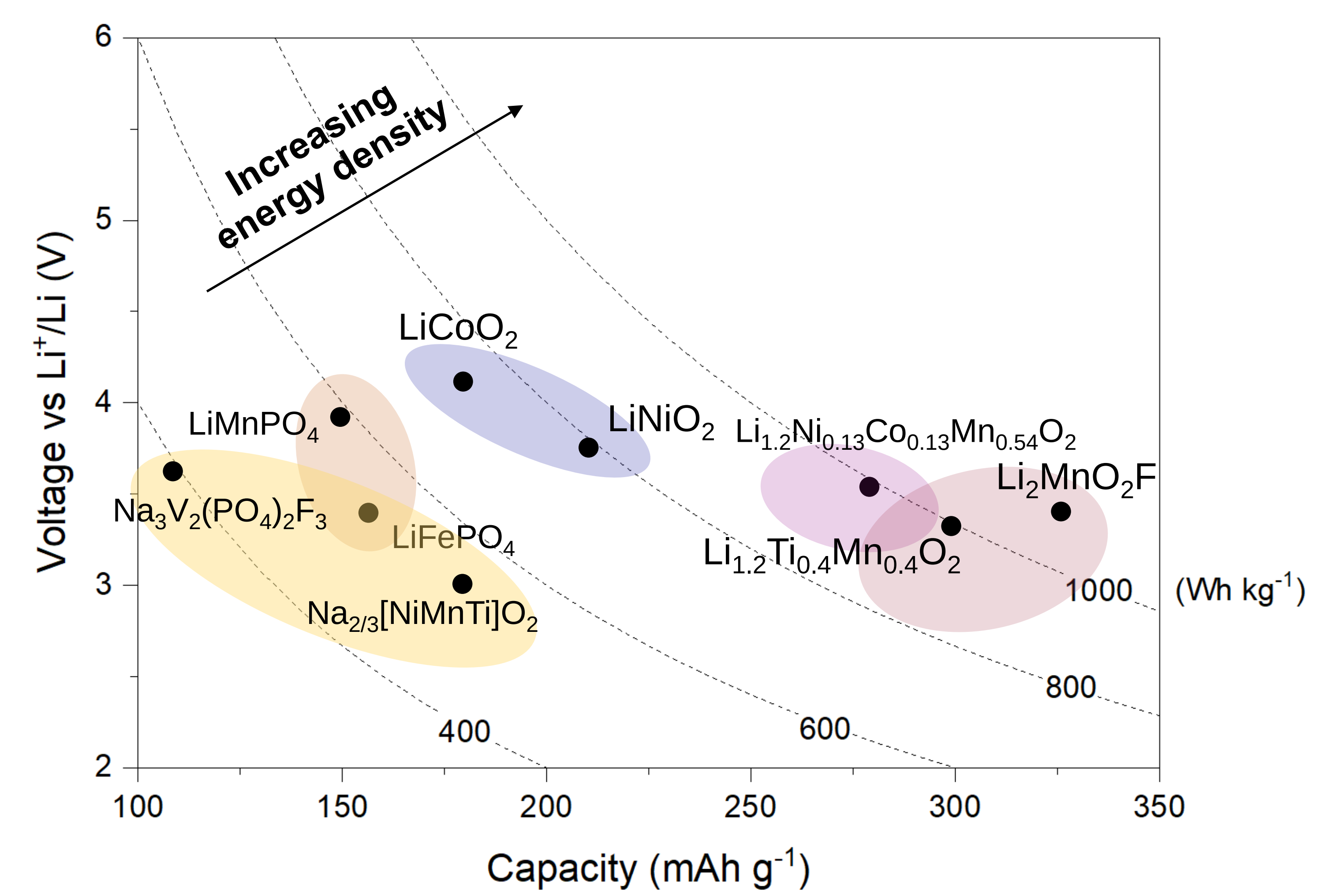
Na-ion batteries

The good…

	Li^+	Na^+
Cell cost ($/kWh)	150	**50**
Abundance (ppm)	20	**23,000**
Safety risk	High	**low**

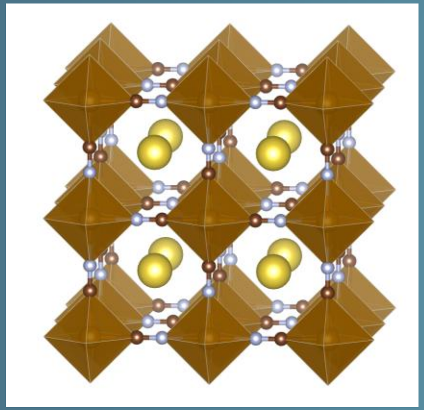
The bad…

	Li^+	Na^+
Ionic radius (Å)	**0.76**	1.02
molar mass (g mol^{-1})	**7**	23
Reduction potential (V)	**-3.05**	-2.71



Na-ion battery cathodes

Prussian Blue/White analogues



High power

Very low cost

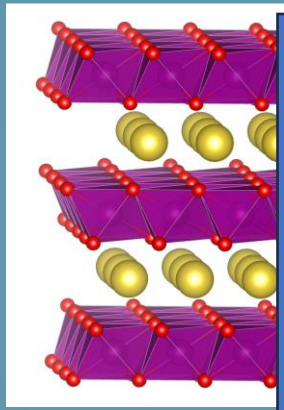
Very good lifetime

Natron Energy

Altris

CATL

Layered oxides



High energ

Moderat

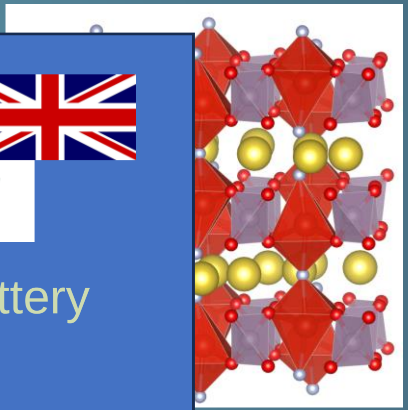
Good lif

faradion

CATL

HiNa BATTERY

Polyanion



igh power

erate cost

d lifetime

TIAMAT

LiNa Energy

Solid state $Na/NiCl_2$ battery

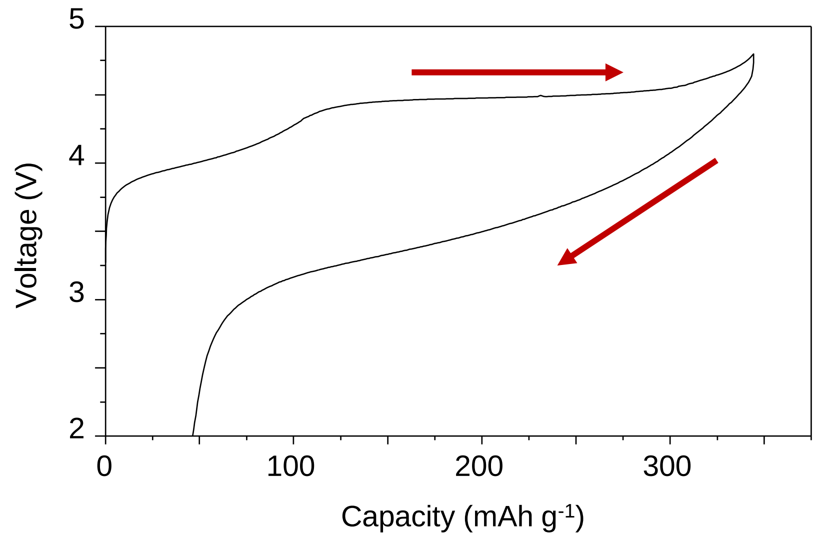
$50/kWh

160℃ - 300℃ operating temp

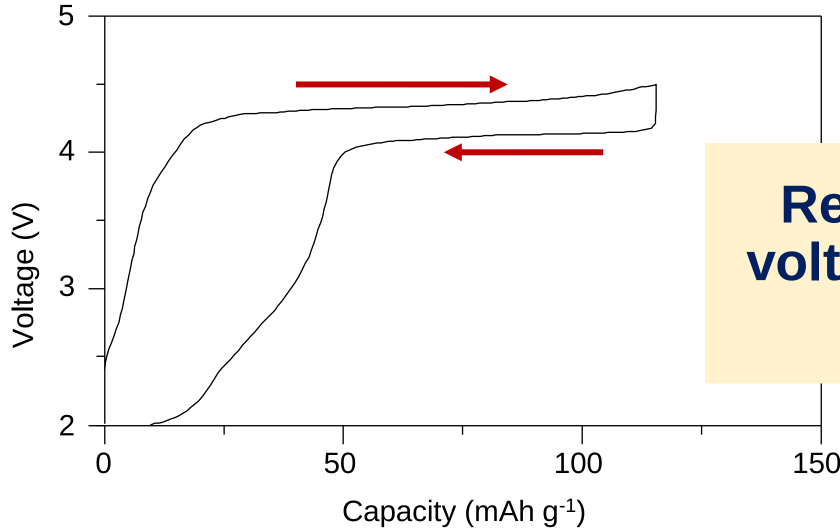
Utility and heavy duty transport

Innovation in Na-ion cathodes

$Li_{1.2}Ni_{0.13}Co_{0.13}Mn_{0.54}O_2$

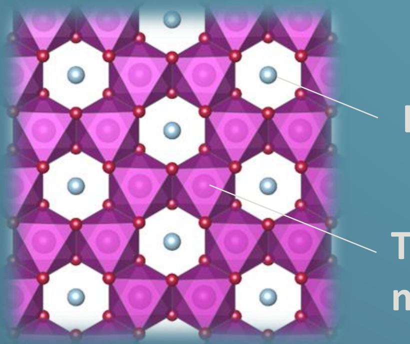


$Na_{0.6}Li_{0.2}Mn_{0.6}O_2$

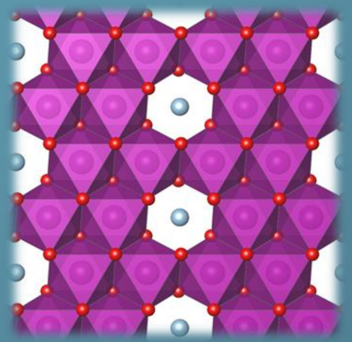


Reversible high voltage O-redox is possible

Honeycomb



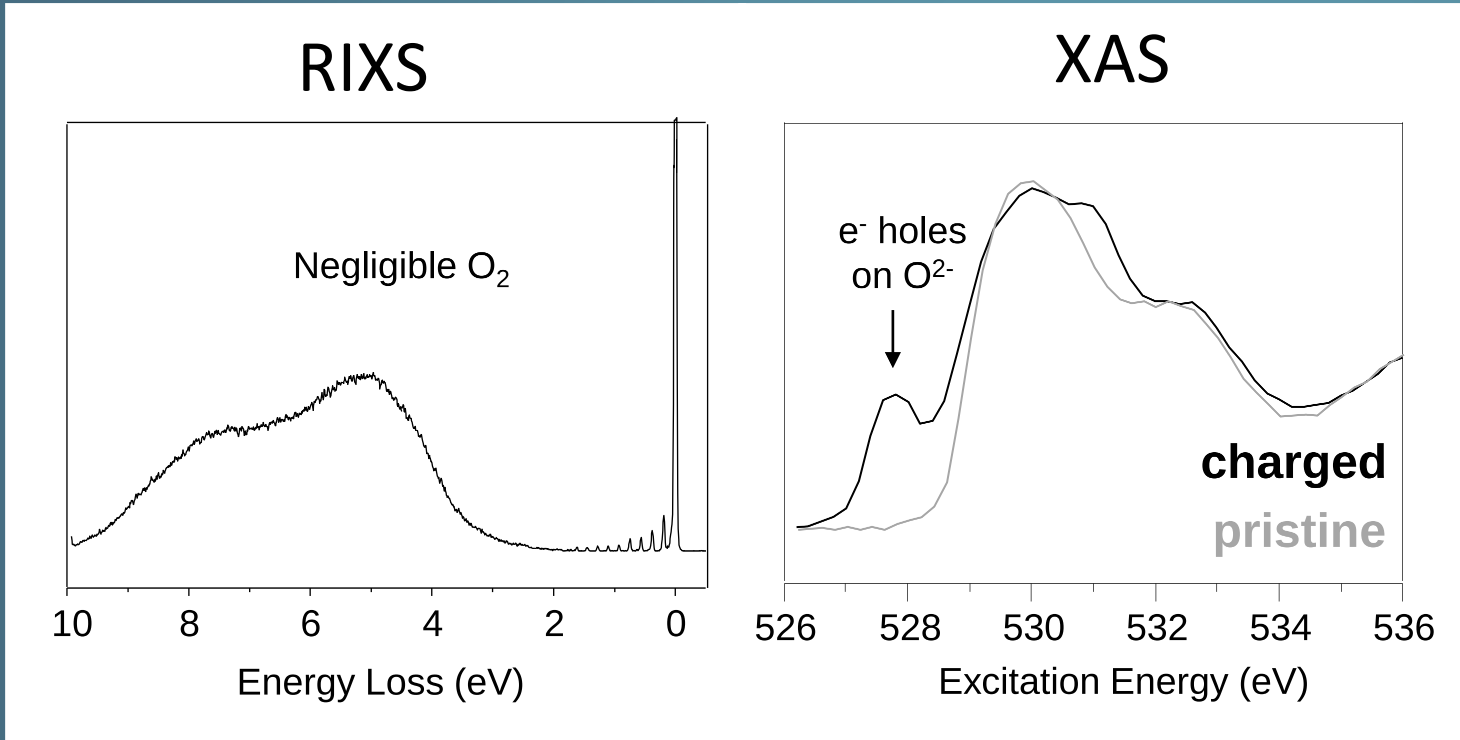
Ribbon



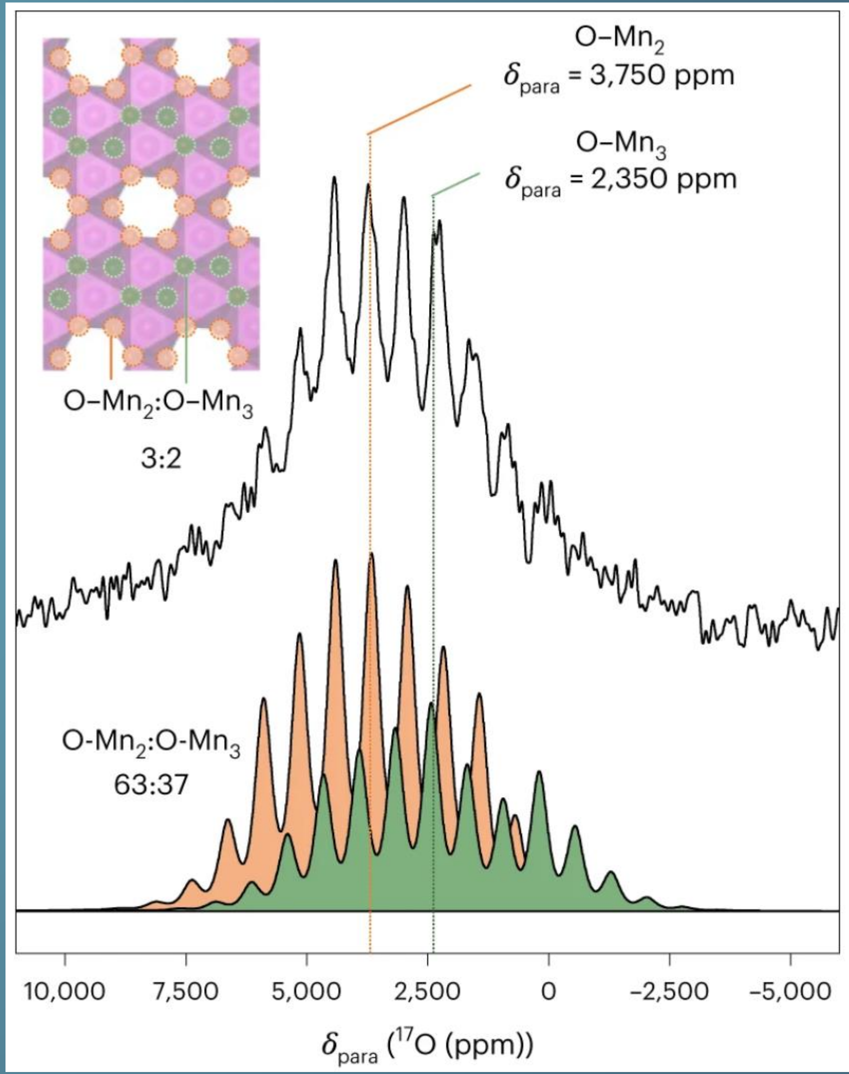
Atomic-scale control can lead to real and significant improvements

House et al. *Nature* **577**, 502-508 (2020)

Innovation in Na-ion cathodes



^{17}O NMR



O_2 formation suppressed

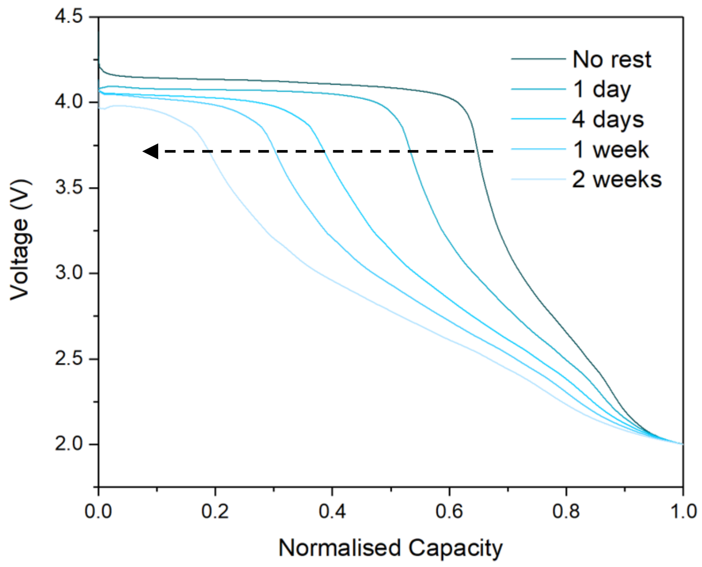
Stable electron holes on O^{2-}

House et al. *Nature Energy* **8**, 351–360 (2023)

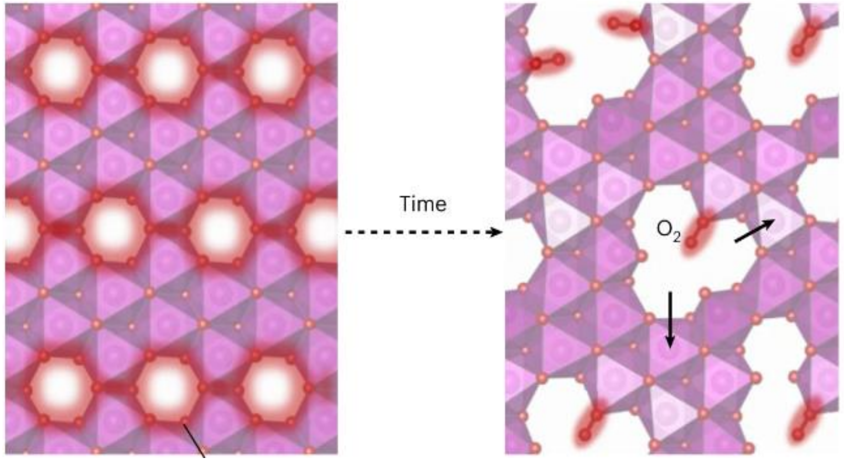
Innovation in Na-ion cathodes

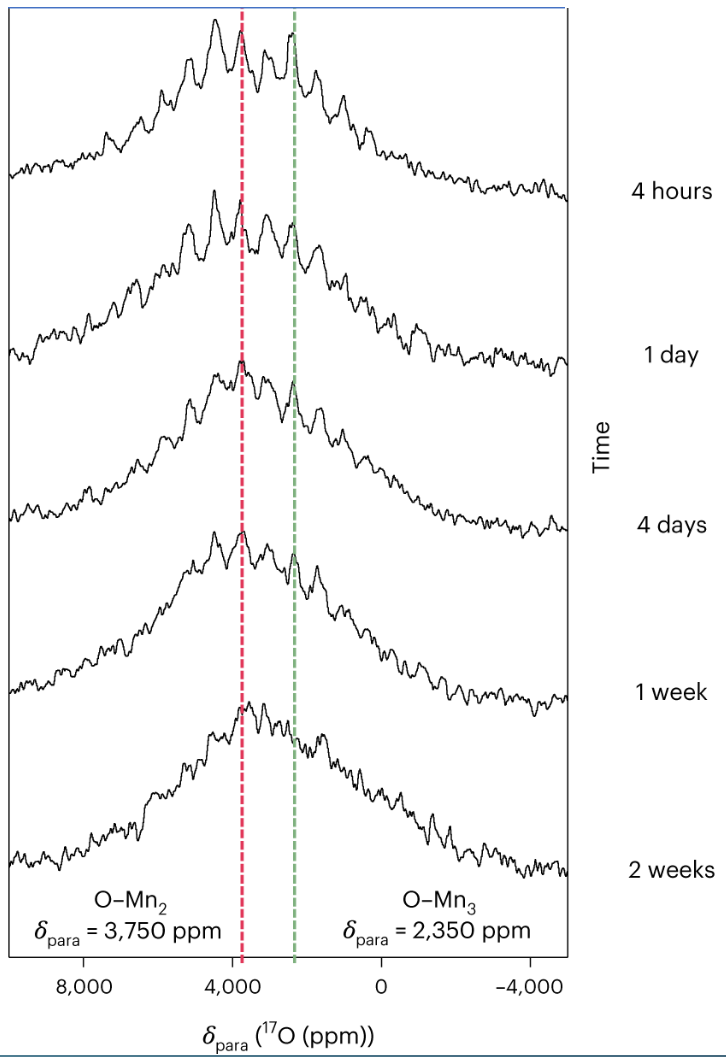
^{17}O NMR

Charge to 4.5V, **rest for *x* days**, then discharge



Track and understand the stability of these high voltage materials





House et al. *Nature Energy* **8**, 351–360 (2023)

Na-ion for electric vehicles?

- Low cost < £10k
- 150-250 mile range
- 15-20 min fast charging
- Safer shipping at 0 V
- Earth-abundant raw materials

BYD

30kWh Na-ion battery
190-mile range
RMB 78,000
(£8,800)

Na 中科海钠 HiNa BATTERY
JAC 江淮汽车

25kWh Na-ion battery
155-mile range
RMB 46,900 – RMB 76,400
(£5,300 - £8,600)

Closing thoughts

- Battery energy storage critical to vehicle electrification (& potentially grid and aviation too)
- Li-ion → lower cost, higher energy density
  - Cathode material a significant expense and performance limit
  - Lithium-rich cathodes & disordered rocksalts
  - Harness oxygen redox chemistry by suppressing O_2
- Na-ion is here to stay
  - Low-mid range commuter EVs
  - Materials innovation + economic headwinds will determine extent of market penetration

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- **Prof. Sir Peter Bruce & Group**
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- **Prof. Rob Weatherup & Group**
- **Prof Mauro Pasta & Group**

CATMAT

THE FARADAY INSTITUTION

NEXGENNA

UKRI Science and Technology Facilities Council | ISIS Neutron and Muon Source

diamond

faradion

AMTE POWER

THE FARADAY INSTITUTION

UKRI Engineering and Physical Sciences Research Council

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