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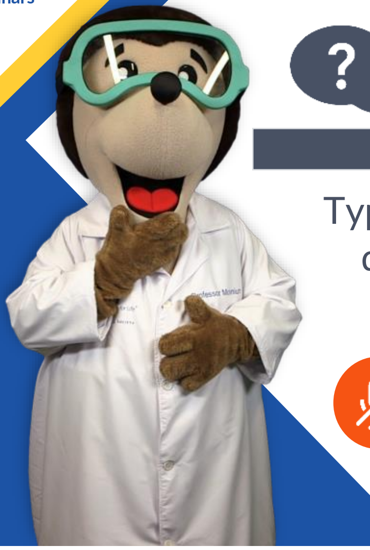

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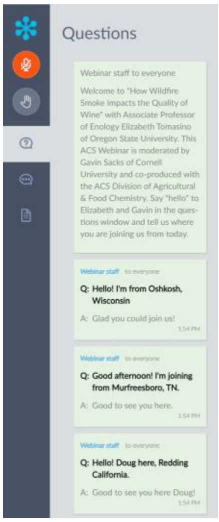

Questions

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Webinar staff to everyone

Q: Hello! I'm from Oshkosh, Wisconsin

A: Glad you could join us!

1:54 PM

Webinar staff to everyone

Q: Good afternoon! I'm joining from Murfreesboro, TN.

A: Good to see you here.

1:54 PM

Webinar staff to everyone

Q: Hello! Doug here, Redding California.

A: Good to see you here Doug!

1:54 PM

"Why am I muted?"
Don't worry. Everyone is muted except the Presenter and the Host. Thank you and enjoy the show.

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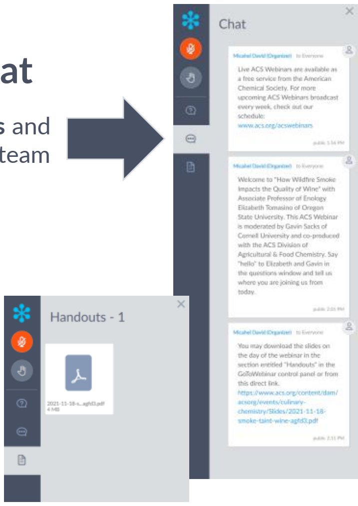

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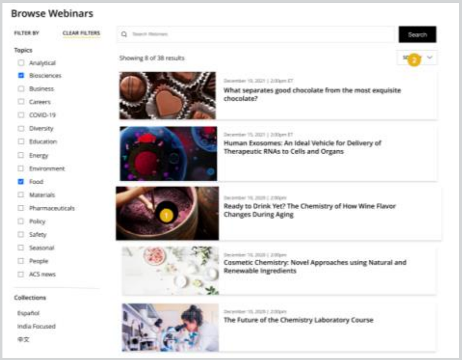

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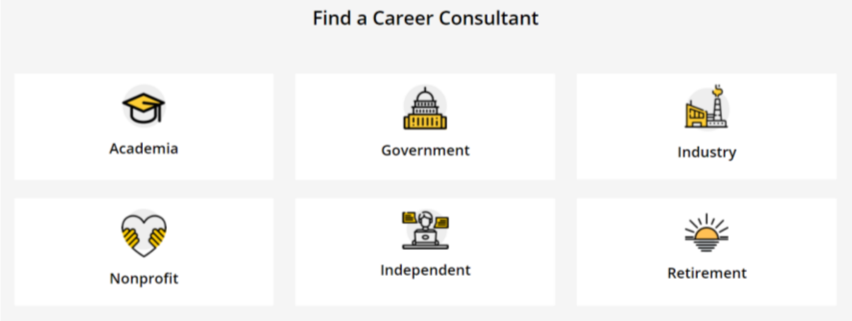

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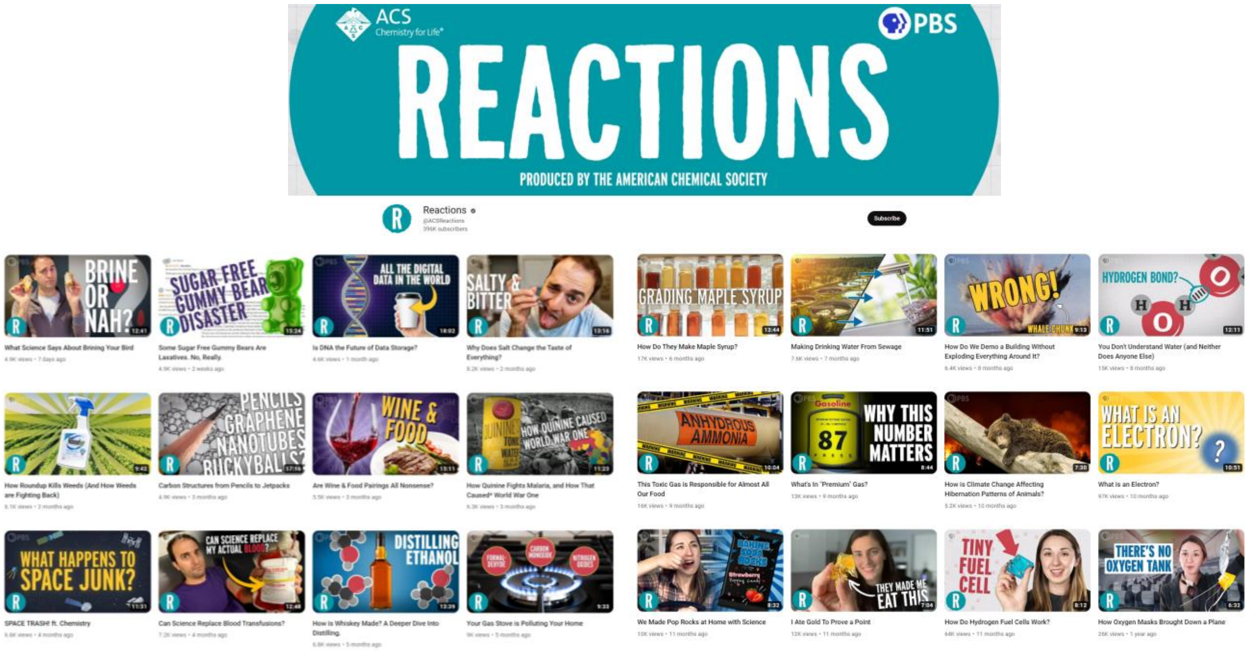

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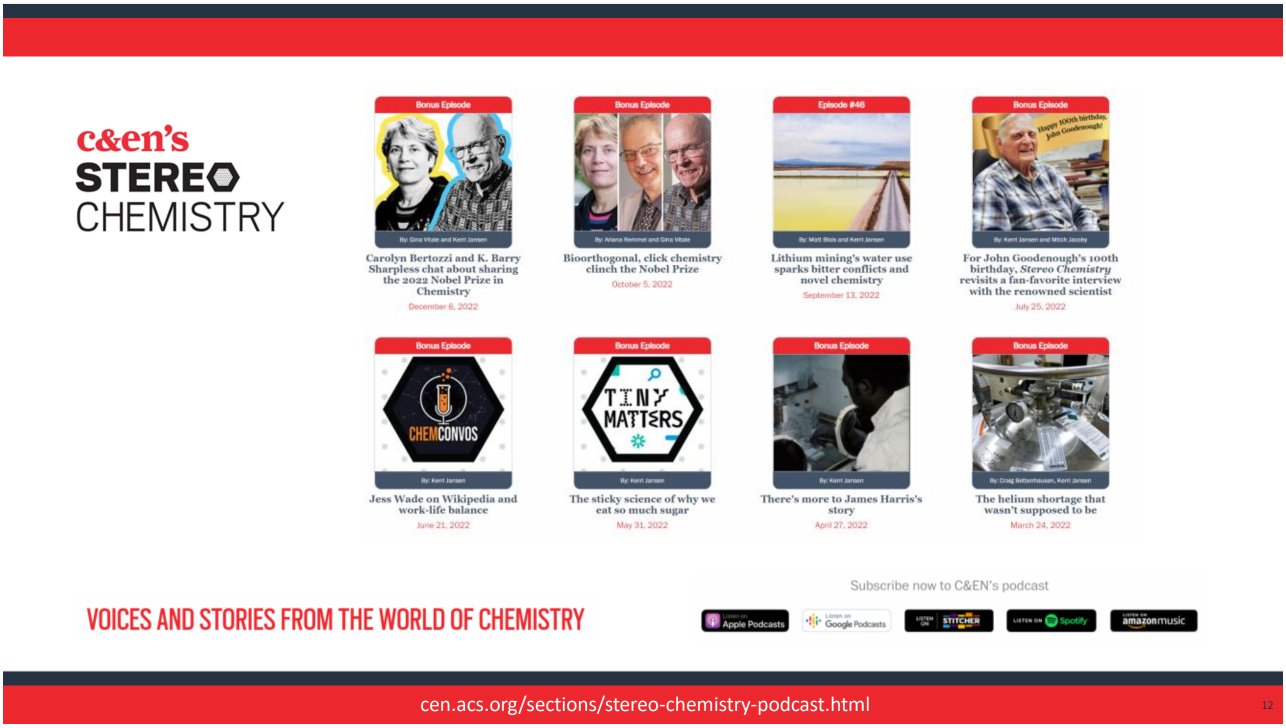

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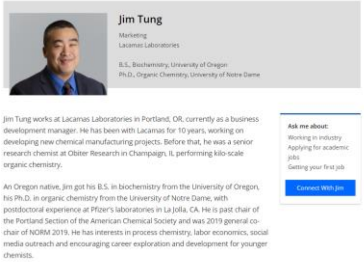

Jim Tung

Marketing
Lacamas Laboratories

B.S., Biochemistry, University of Oregon
Ph.D., Organic Chemistry, University of Notre Dame

Jim Tung works at Lacamas Laboratories in Portland, OR, currently as a business development manager. He has been with Lacamas for 10 years, working on developing new chemical manufacturing projects. Before that, he was a senior research chemist at Obiter Research in Champaign, IL performing kilo-scale organic chemistry.

An Oregon native, Jim got his B.S. in biochemistry from the University of Oregon, his Ph.D. in organic chemistry from the University of Notre Dame, with postdoctoral experience at Pfizer's laboratories in La Jolla, CA. He is past chair of the Portland Section of the American Chemical Society and was 2019 general co-chair of NORM 2019. He has interests in process chemistry, labor economics, social media outreach and encouraging career exploration and development for younger chemists.

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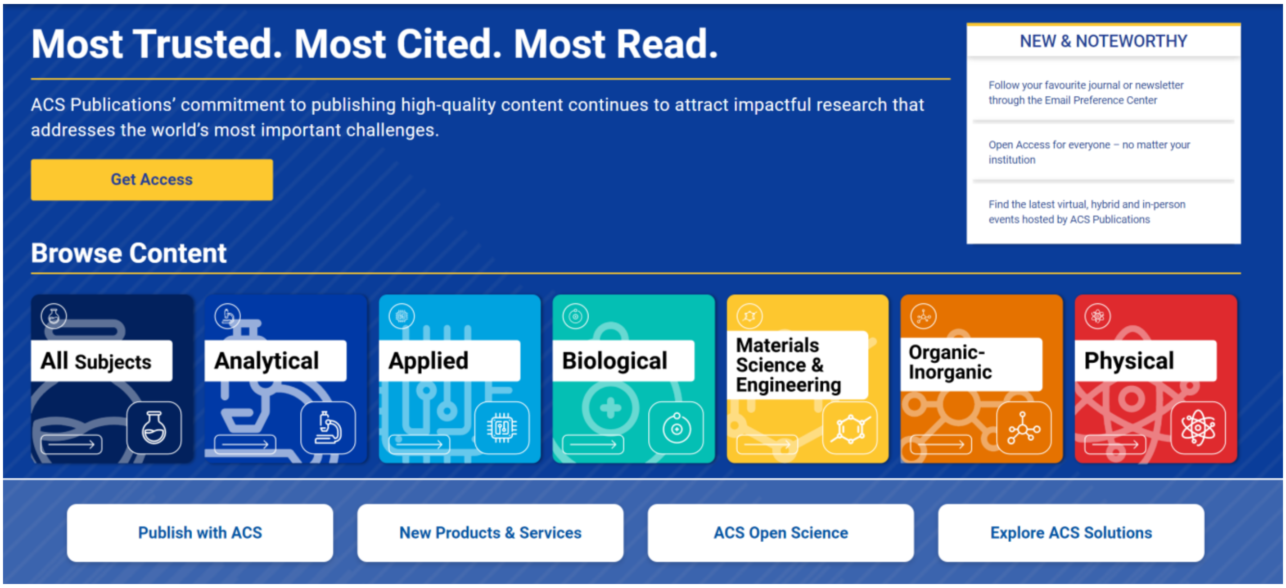

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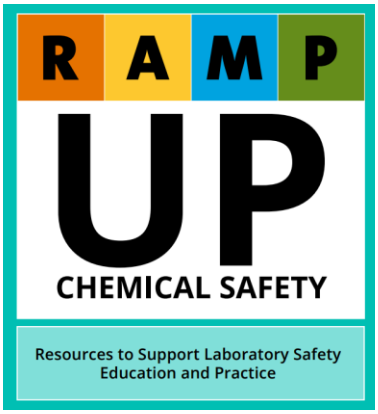

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Advancing ACS' Core Value of Diversity, Equity, Inclusion and Respect

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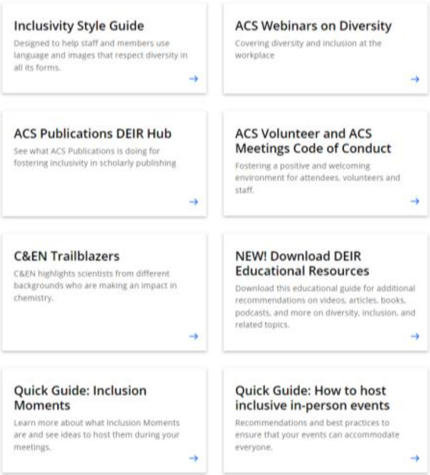

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Diversity, Equity, Inclusion, and Respect

**Adapted from definitions from the Ford Foundation Center for Social Justice:

Equity**
Seeks to ensure fair treatment, equality of opportunity, and fairness in access to information and resources for all. We believe this is only possible in an environment built on respect and dignity. Equity requires the identification and elimination of barriers that have prevented the full participation of some groups.

Diversity**
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Inclusion**
Builds a culture of belonging by actively inviting the contribution and participation of all people. Every person's voice adds value, and ACS strives to create balance in the face of power differences. In addition, no one person can or should be called upon to represent an entire community.

Respect
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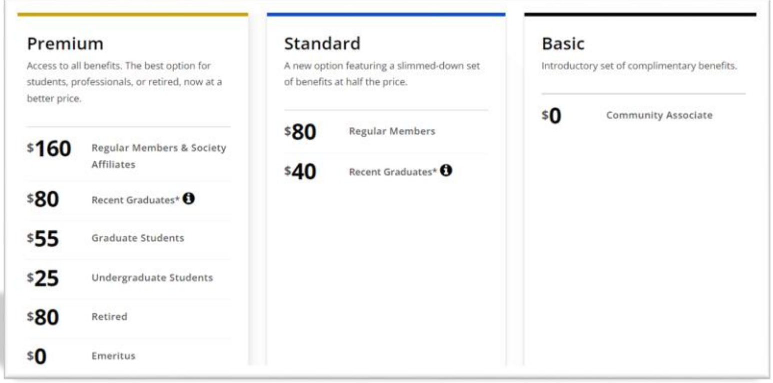

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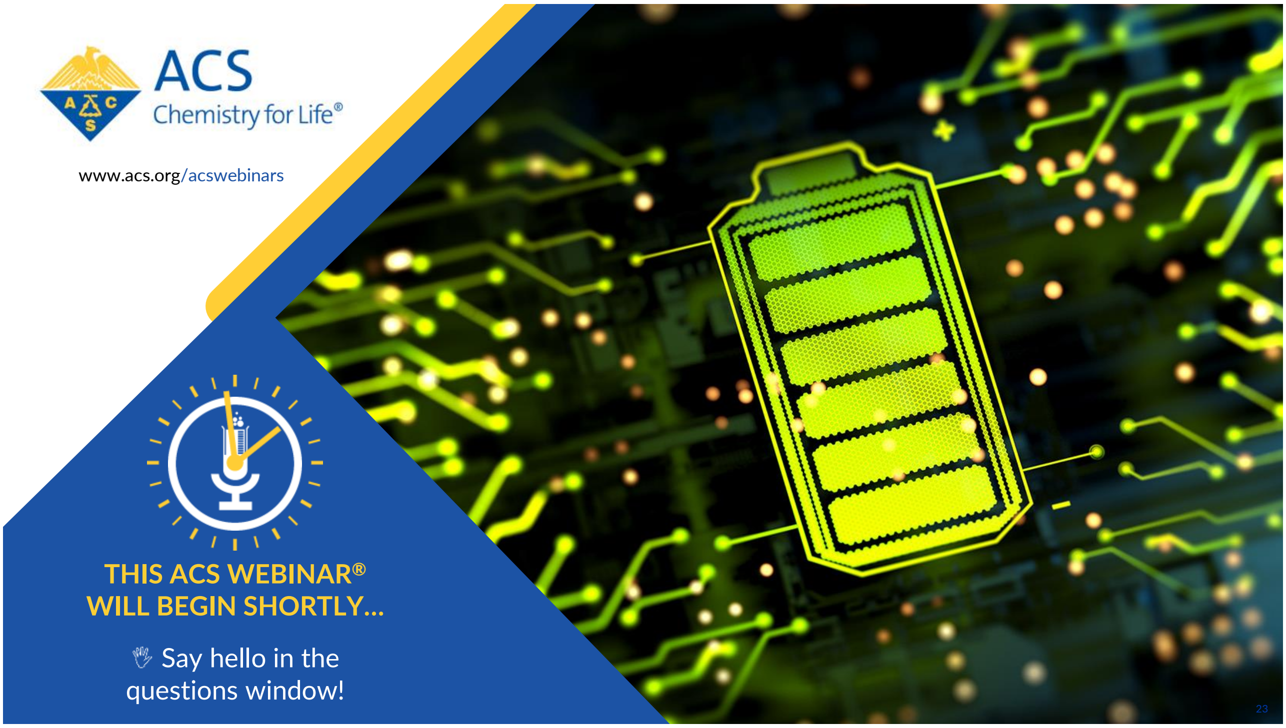

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Powering the Future: The Latest Battery Technologies

SERGIY KALNAUS, PhD	**ERIK G. HERBERT, PhD**	**NIAN LIU, PhD**	**BILL TUSZYNSKI, PhD**
Senior Staff Scientist, Oak Ridge National Laboratory	Senior Staff Scientist and Mechanical Properties and Mechanics Group Lead, Oak Ridge National Laboratory	Assistant Professor, School of Chemical and Biomolecular Engineering, Georgia Tech	Partner, The Unami Group, LLC

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Solid-state batteries – why mechanics is critical?

Sergiy Kalnaus

kalnauss@ornl.gov

03/14/2024

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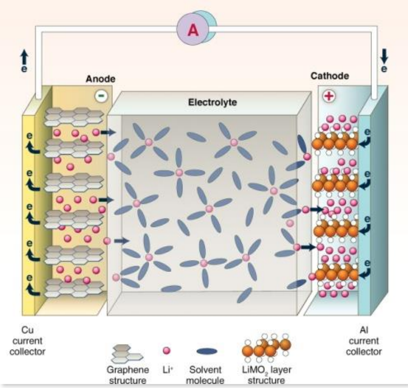
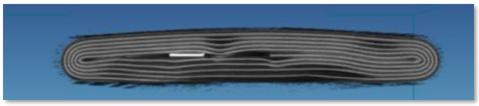
---

Conventional Li-ion batteries

- Anode: graphite with binder
- Cathode: layered metal oxide with binder
- Charge carried by ions through electrolyte
- Electrolyte: Li salt in organic solvents
- Separation of electrodes in space: porous polymer separator

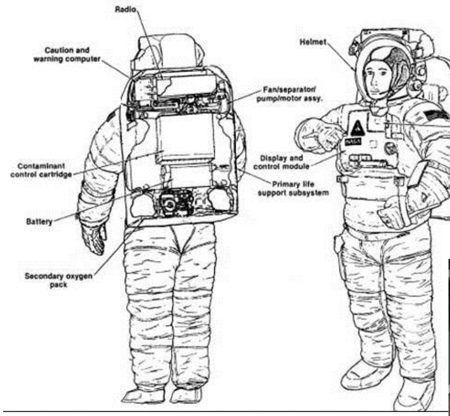


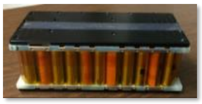


Wang, D., et al., J Power Sources 140 (2005) 125-28

Examples of usage

- NASA spacesuit
- Wearable in military – flexible vest



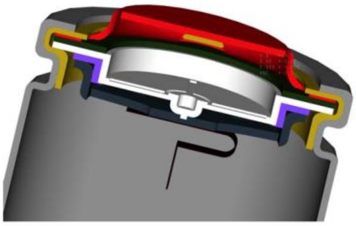


Q: What is EMU?

https://ntrs.nasa.gov/
https://www.army.mil/
Roller, D.P., Slane, S., 1998 IEEE, **DOI:** 10.1109/BCAA.1998.653843

Limitations of conventional Li-ion batteries

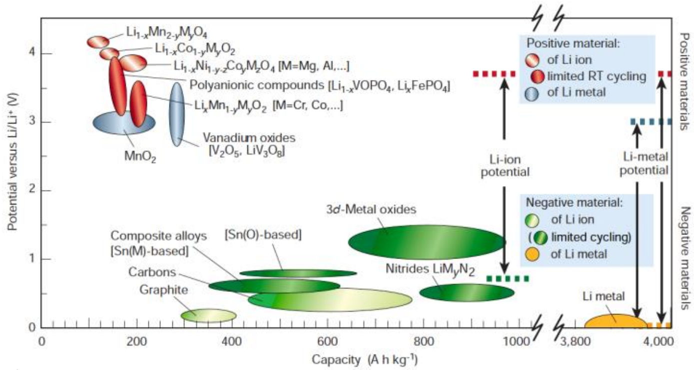
- Liquid electrolyte: fire hazard, toxic, voltage window, leakage, transference number
- Safety issues/devices



https://ntrs.nasa.gov/
http://cnn.com

Advantages of solid-state batteries

- Wider temperature operating range and stability
- No electrolyte to burn or gas
- Abuse tolerance to overcharge since no gas produced
- Higher voltages ($LiMn_{1.5}Ni_{0.5}O_4$ – 4.9V)
- Reimagine packaging
- Wearable technologies
- Structural batteries

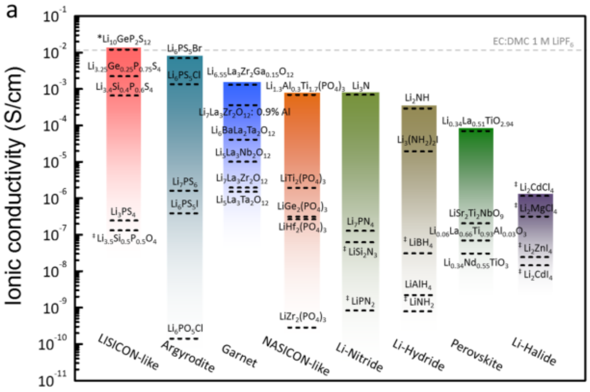


J.M. Tarascon, M. Armand, Nature, 414, 15 (2001) 359

Solid electrolytes

- Solid electrolyte – ceramics, or glass
- Possibility to include metallic lithium anode

LiI solid electrolyte cell for pacemakers



Q: When was the first solid electrolyte invented?

Schneider, A., et al. J Power Sources 5 (1980), 15-23
Takada, K, Acta Materialia 61 (2013), 759-770

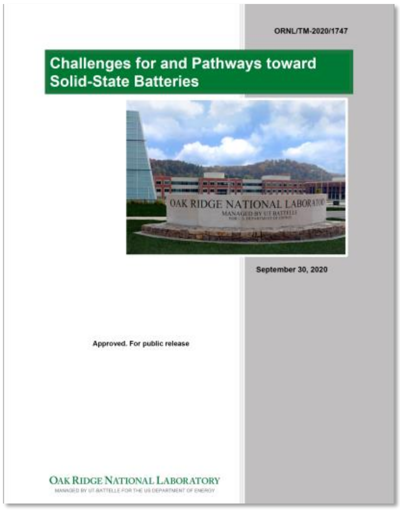
Solid state uphill battle

- Quantum Scape
- Factorial Energy
- Solid Power
- LG Chem
- Samsung SDI
- Toyota
- …

Date for large scale production keeps shifting

2024 2027 2030 ?

Where do we stand?



ORNL/TM-2020/1747

Challenges for and Pathways toward Solid-State Batteries

September 30, 2020

Approved. For public release

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Challenges for and Pathways toward Li-Metal-Based All-Solid-State Batteries

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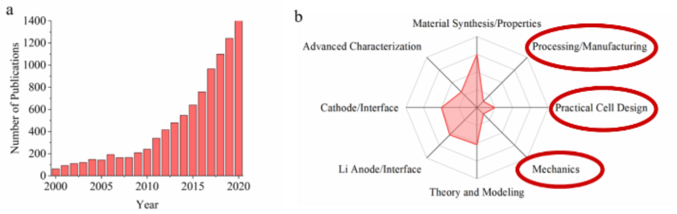
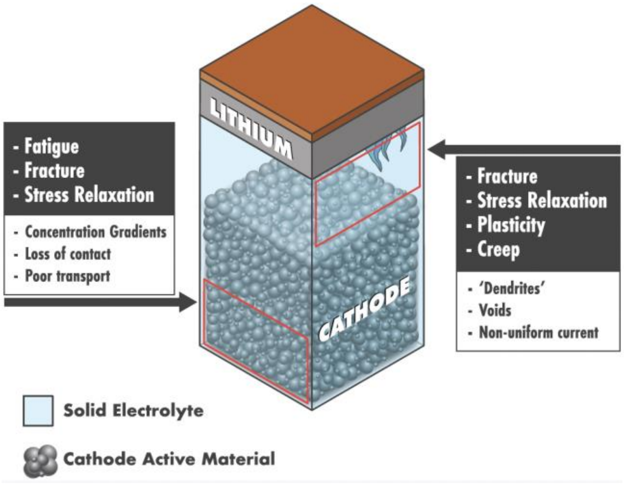


What distinguishes SSBs from liquid e-lyte counterpart?

- Micrometers of lithium can be plated and stripped on the anode side;
- Lithium can plate INSIDE the electrolyte;
- Lithium plating into the electrolyte creates the competition for stress relief;
- Fracture of cathode particles immersed in liquid electrolyte leads to increase in s/a of cathode; in solid electrolyte it leads to loss of contact;

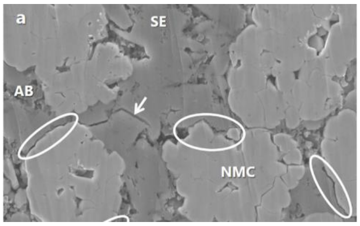


Sources of stress in SSB

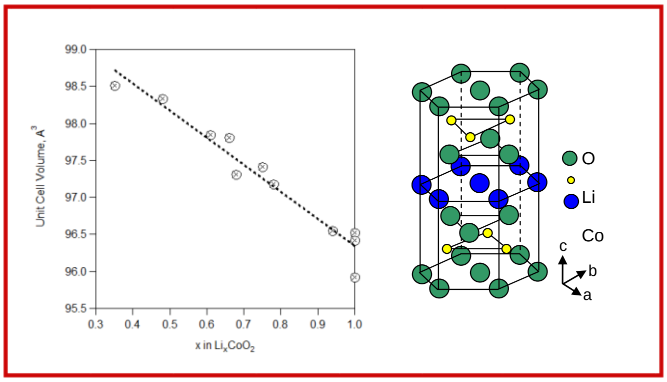

Compositional Strain in Cathode

External Pressure

Stress From Plated Lithium

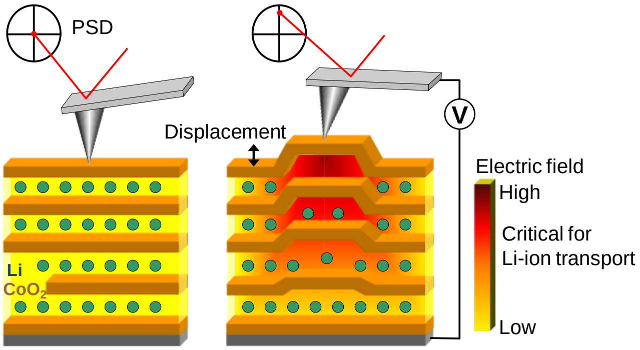


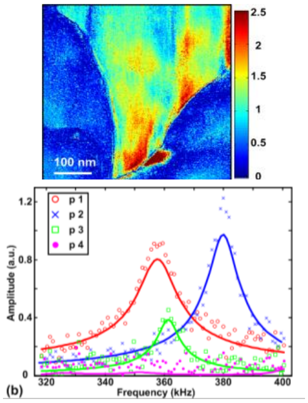
M. Yamamoto, et. al J Pow. Sources 473 2020



Electrochemical Strain Microscopy

Concept: Utilize volume changes as function of Li-ion concentration

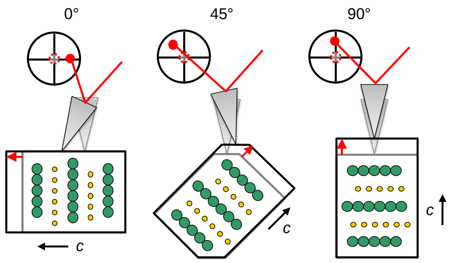




- The local Li-ion concentration can be changed by the application of a local bias.
- The higher the Li-ion mobility, the higher the induced surface displacement.

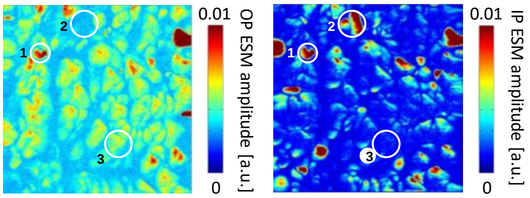
Balke, N., Kalnaus, S., Daniel, C., Jesse, S., and Kalinin, S.V., 2012, "Local Detection of Activation Energy for Ionic Transport in Lithium Cobalt Oxide," Nano Letters, 12(7) pp. 3399-3403.

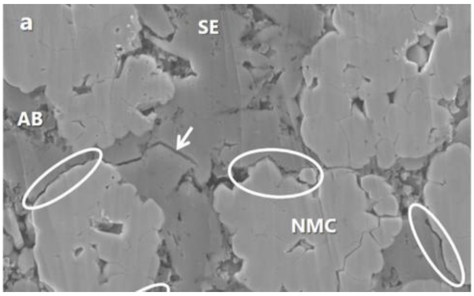
Orientation dependence



The mobility of lithium and the compositional strains are highly heterogeneous in cathode. Electrolyte should remain functional over many cycles subjected to stresses from cathode.

OTHERWISE…

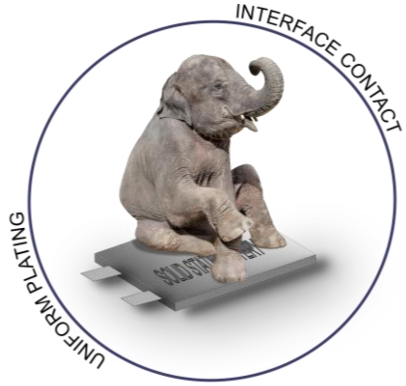




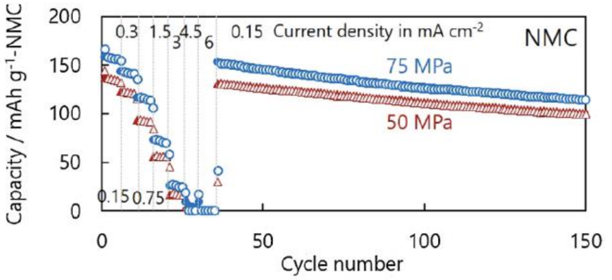
Balke, N., Eliseev, E.A., Jesse, S., Kalnaus, S., Daniel, C., Dudney, N.J., Morozovska, A.N., and Kalinin, S.V., 2012, "Three-Dimensional Vector Electrochemical Strain Microscopy," Journal of Applied Physics, 112, 052020.

Sources of stress in SSB

Compositional Strain in Cathode ↔ **External Pressure** ↔ **Stress From Plated Lithium**



10s of MPa compared to ~ 0.05 MPa in conventional battery modules

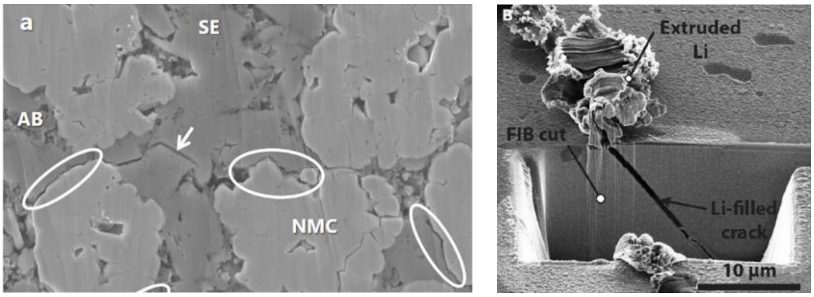


M. Yamamoto, et. al J Pow. Sources 473 2020

Sources of stress in SSB

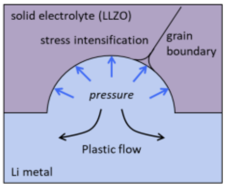
Compositional Strain in Cathode ↔ **External Pressure** ↔ **Stress From Plated Lithium**

If inelastic strain is not triggered, the result is stress relief by fracture



Stress buildup can be relieved by:

- Inelastic flow in lithium
- Inelastic flow in electrolyte
- Fracture

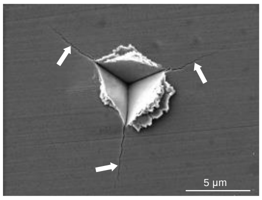


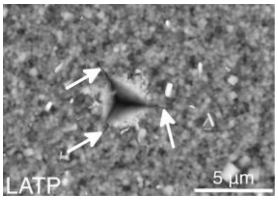
M. Yamamoto, et. al J Pow. Sources 473 2020
E. Kazyak et al Matter 2, 1025–1048, 2020

Solid electrolyte should deal with the stress

But here's the problem …

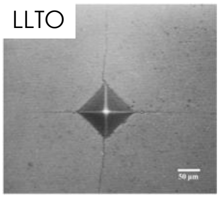
NASICONs

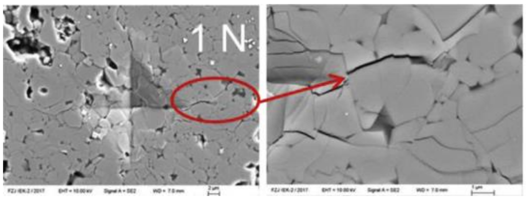




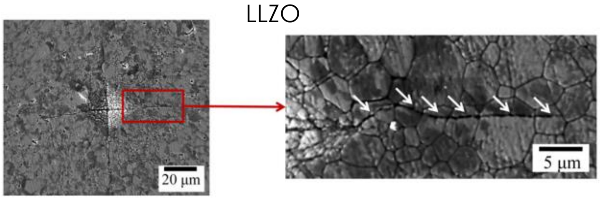
LATP

LLTO





LLZO



J. Wolfenstine et al. J Mater Sci 47 2012
Y. Kim et al J Am Ceram Soc 99(4) 2016
S. Kalnaus et al ACS Appl Energy Mater 4, 2021 11684
S. Kalnaus et al JMR 36(4) 2021

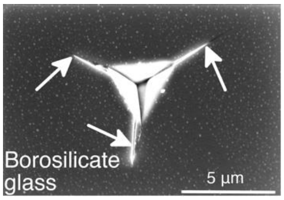
Glasses are more interesting

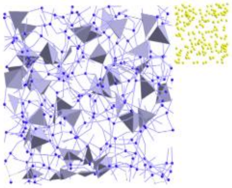
Amorphous or glassy materials are unusual because they can deform without conserving the volume.

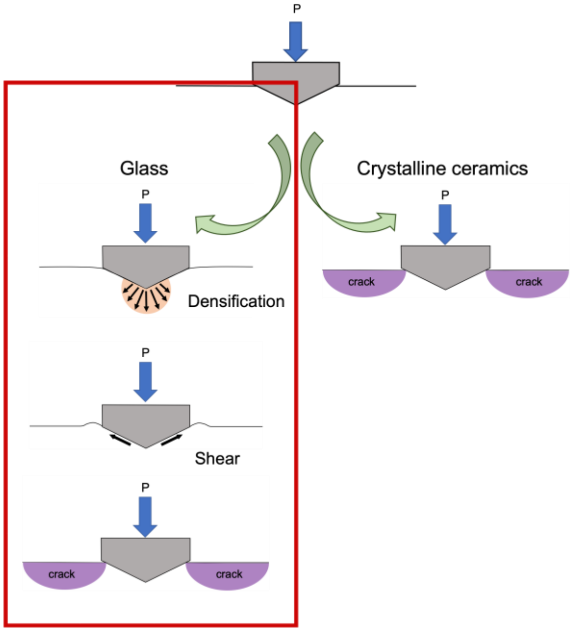
Mechanisms to reduce stress:

- densification
- isochoric shear
- fracture

Many binary and ternary glasses are still brittle







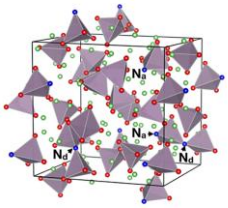
S. Kalnaus et al JMR 36(4) 2021
F. Michel et al J Non-Cryst Solids 379 2013.

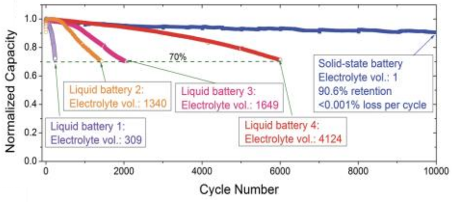
ORNL is working on ionic glasses

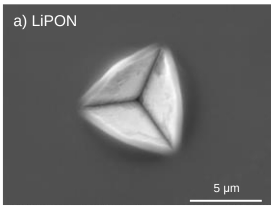
- Inverted glass, or “high modifier” glass
- Lower viscosity
- Higher ionic conductivity
- Mechanical behavior similar to BMGs

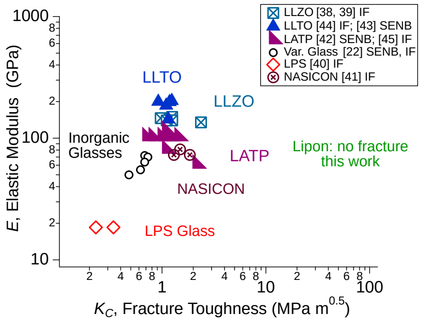
Good example - LiPON

$Li_xPO_yN_z$
$x = 2.9\text{-}3.1$
$y = 3.3\text{-}3.8$
$z = 0.14\text{-}0.16$









J. Li, et. al. Adv Energy Mater 5, 2015
V. Lacivita, et al Cnem Mater 30, 2018
H.J.L. Trap, J.M. Stevels, Physical properties of invert glasses, Glastech. Ber. 5, 1959.

Conclusions and outlook

- 100+ years of solid state ionics
- Upscaling to large format is “production hell”
- Making SSBs with old approaches from liquid electrolyte batteries requires enormous pressures to make battery working
- Electrolyte is key component
- Glass ionic conductors are worth exploring as they provide several mechanisms to avoid fracture + no grain boundaries, pores, voids, etc.
- How to deal with metallic lithium and “dendrites”?

Acknowledgement

- **ORNL LDRD Program**
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U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

U.S. Department of Transportation

Questions?

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Mechanics of Solid-State Battery Materials:
Hidden Surprises of Lithium Metal

Erik G. Herbert
Sergiy Kalnaus
Andrew S. Westover
Nancy J. Dudney
Stephen A. Hackney (MI Technological University)

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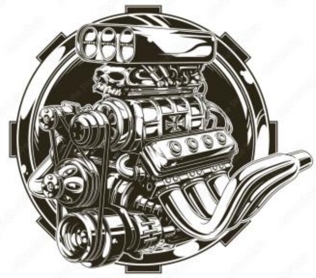
THE MECHANISM OF ACTION

Befriended Alien
- Knows about burning gasoline
- Fills the passenger compartment with gas

https://www.dreamstime.com/illustration/alien-gas-station.html



https://stock.adobe.com/search/images?k=cartoon+car+exhaust&asset_id=119337670

Mechanism of Action
- Basis of informed decision making
- Prevents unexpected or undesirable outcomes

https://stock.adobe.com/search/images?k=cartoon+car+exhaust&asset_id=337262281

THE STRENGTH OF METALS

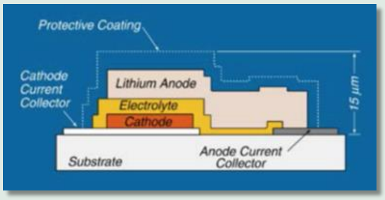
TRUE or FALSE?

The strength of a metal is an intrinsic material property.

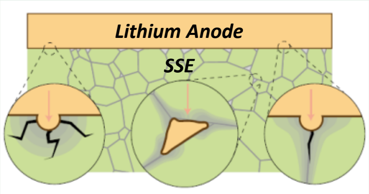
(a) TRUE, because the strength of a metal is uniquely controlled by the ***bonding*** between the metallic ion cores, which is independent of the processing conditions.

(b) FALSE, because strength depends on ***defects*** and defects can be controlled through processing.

SSBs: The critical role of mechanics



J.B. Bates *et al.*, Solid State Ionics **135** (2000)



T. Famprikis *et al.*, Nature Materials 18 (2019)

- Nonuniform transport of Li^+ generates localized gradients in elastic strain
- Strain creates stress, σ
- $\sigma = f$ *(length scale, strain rate, temp., cycling, …)*
- $\sigma = f$ *(operational efficiency of the dominant stress relief mechanism)*
- *σ drives fracture of the SSE*

Mechanical Properties

★ ***Predictive capability:*** *Quantify the material's response when its boundaries are mechanically loaded*

★ *The conventional basis for materials selection, design, and modelling*

★ ***BULK PROPERTIES CANNOT BE USED TO UNDERSTAND OR SOLVE THE DENDRITE PROBLEM***

Mechanical Behavior

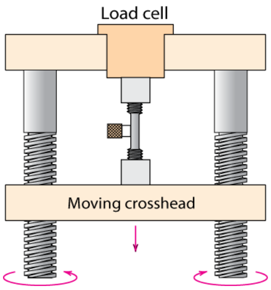
★ ***Elasticity, plasticity, fracture, creep, fatigue, …***

★ *Specific mechanism of action*

★ *Key to engineering structure-property-processing-performance relationships*

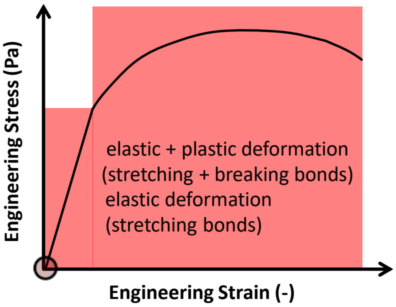
★ ***WHERE WE LOOK TO UNDERSTAND AND SOLVE THE DENDRITE PROBLEM***

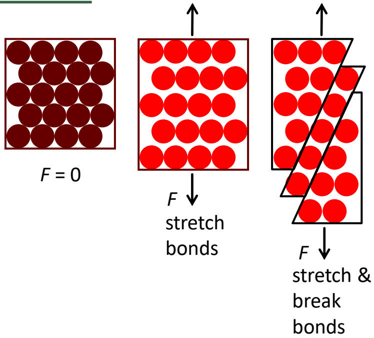
MECHANICAL PROPERTIES



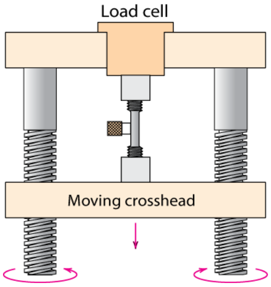
Eng. Stress = F/A_o

Eng. Strain = $\Delta l/l_o$





MECHANICAL PROPERTIES



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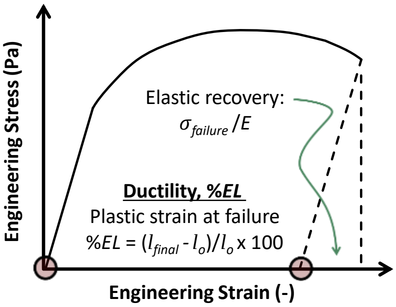
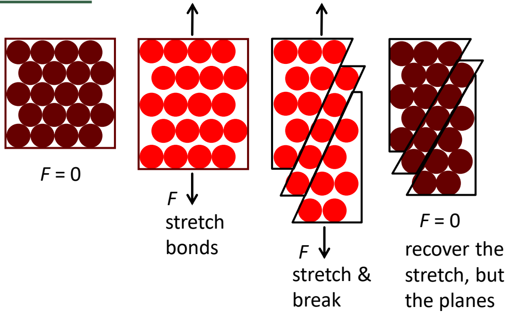
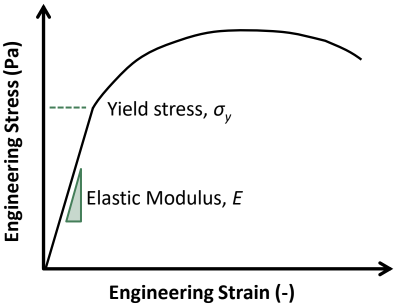




Toughness, *T* (J/m³)
(strain energy density)

$$U_{total} = \int_{\epsilon=0}^{\epsilon_{failure}} \sigma \, d\epsilon$$

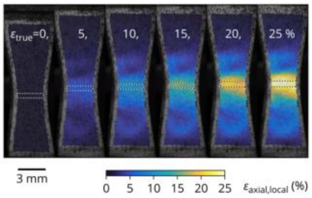


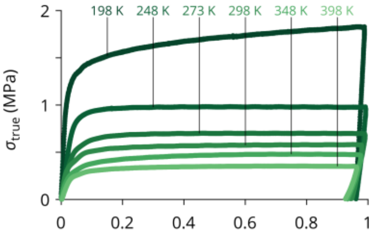
Elastic Modulus, *E* (GPa)
- Intrinsic material property
  $E = f$ (chemistry & composition)
- Elastic regime: How the stress or pressure builds with a change in strain

Yield Stress, σ_y (MPa)
- Extrinsic material property
  $\sigma_y = f$ (chemistry, composition, & *DEFECTS*)
- The threshold stress required to initiate stress relief via plastic deformation

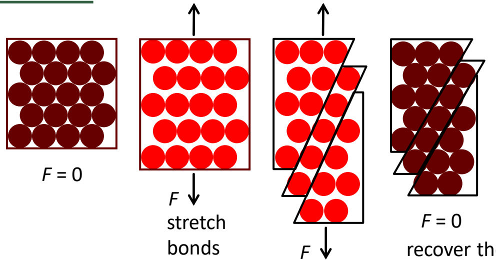
MECHANICAL PROPERTIES

Bulk Lithium Metal Foil





W.S. LePage *et al.*, J. Electrochem. Soc. **166** (2019)



F = 0

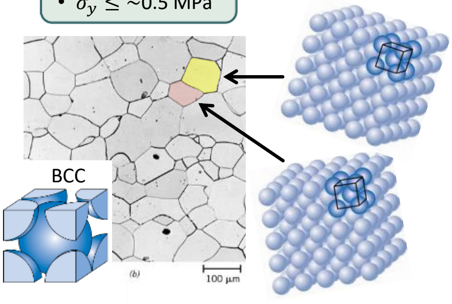
F
stretch bonds

F
stretch & break bonds

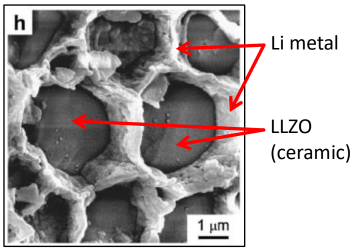
F = 0
recover the stretch, but the planes are still sheared

Bulk Lithium Metal

- $3 \leq E \leq 21$ GPa
- $\sigma_y \leq \sim 0.5$ MPa



Cross-sectioned LLZO cycled to failure



E.J. Cheng *et al.*, Electrochimica Acta **223** (2017)

Lithium Metal: The story of 2 apparent paradoxes

1. How does Li metal support the pressure required to infiltrate the grain boundaries of LLZO?

MECHANICAL PROPERTIES

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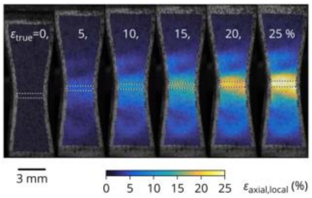

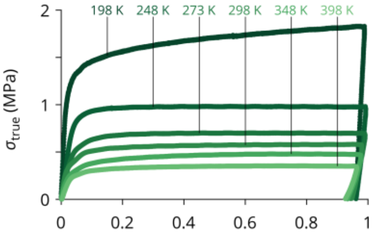

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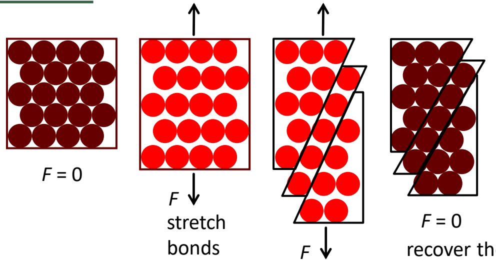

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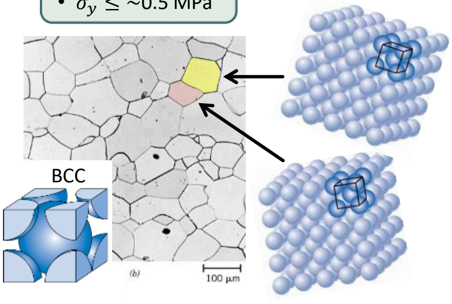
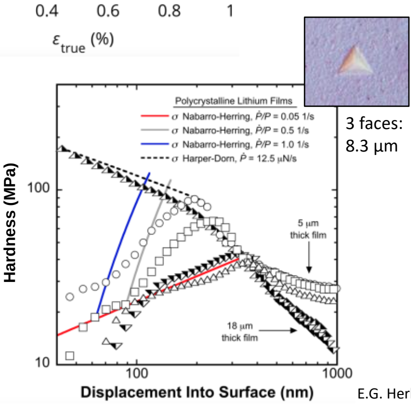


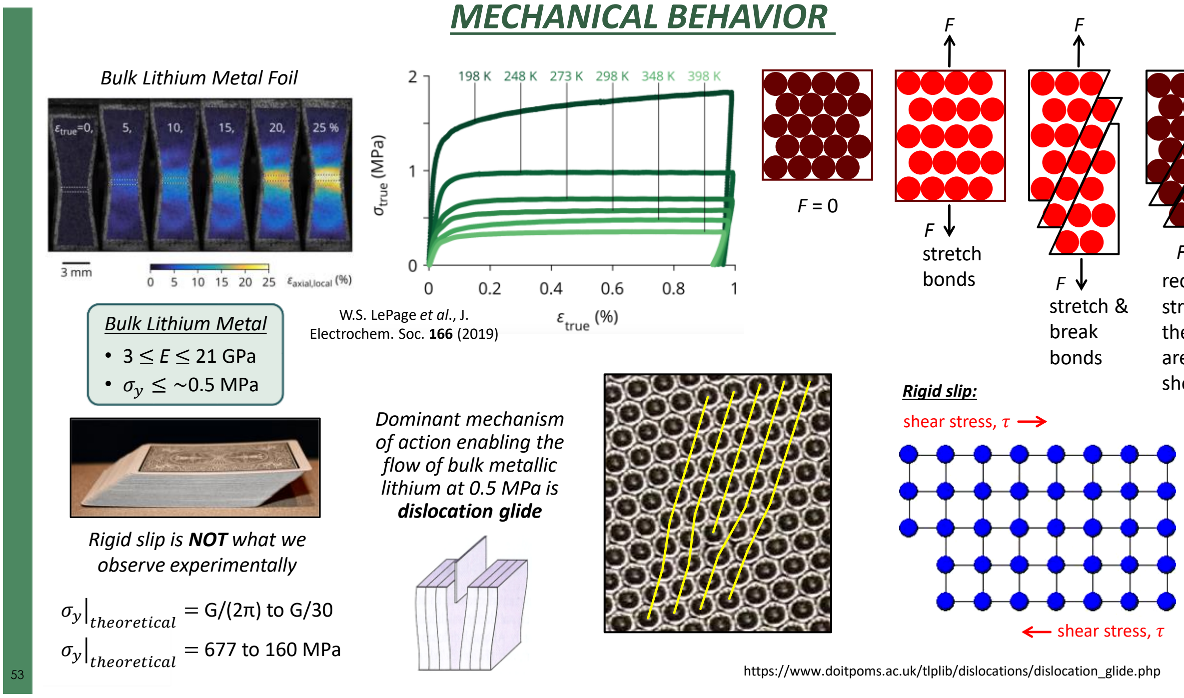


3 faces:
8.3 µm

E.G. Herbert *et al.*, J. Mater. Res., **33** (2018)

Lithium Metal: The story of 2 apparent paradoxes

1. How does Li metal support the pressure required to infiltrate the grain boundaries of LLZO?
2. How does Li metal support pressure $\gg 3\sigma_{flow}$?



MECHANICAL BEHAVIOR

Bulk Lithium Metal Foil

W.S. LePage *et al.*, J. Electrochem. Soc. **166** (2019)

Bulk Lithium Metal
- $3 \leq E \leq 21$ GPa
- $\sigma_y \leq \sim 0.5$ MPa

Rigid slip is ***NOT*** *what we observe experimentally*

$\sigma_y\big|_{theoretical}$ = G/(2π) to G/30

$\sigma_y\big|_{theoretical}$ = 677 to 160 MPa

Dominant mechanism of action enabling the flow of bulk metallic lithium at 0.5 MPa is ***dislocation glide***

F = 0

stretch bonds

stretch & break bonds

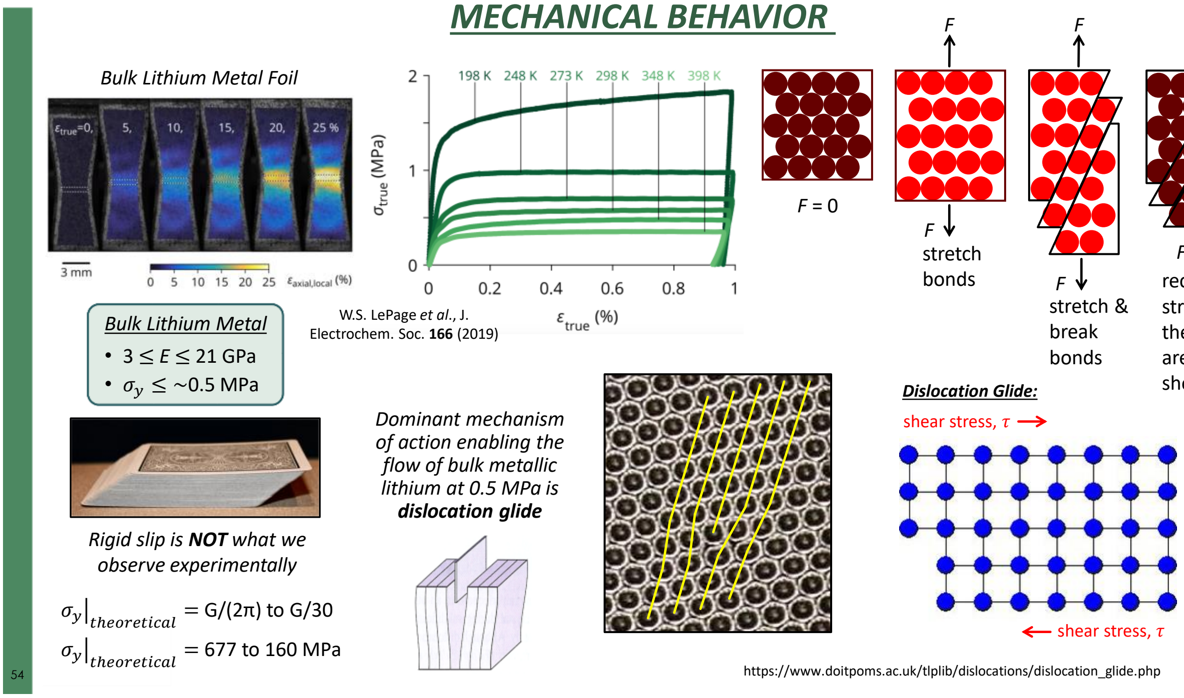
F = 0
recover the stretch, but the planes are still sheared

Rigid slip:

shear stress, τ →

← shear stress, τ

https://www.doitpoms.ac.uk/tlplib/dislocations/dislocation_glide.php



MECHANICAL BEHAVIOR

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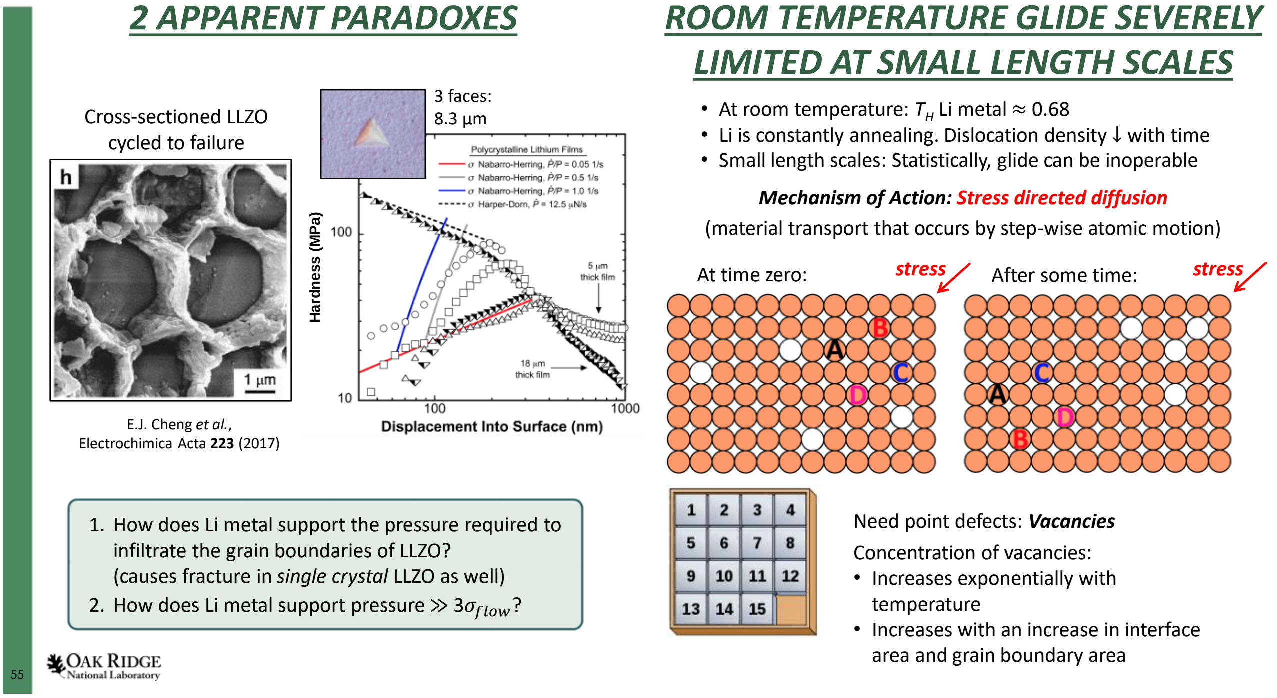


2 APPARENT PARADOXES

Cross-sectioned LLZO cycled to failure

E.J. Cheng *et al.*, Electrochimica Acta **223** (2017)

3 faces: 8.3 µm

1. How does Li metal support the pressure required to infiltrate the grain boundaries of LLZO? (causes fracture in *single crystal* LLZO as well)
2. How does Li metal support pressure $\gg 3\sigma_{flow}$?

ROOM TEMPERATURE GLIDE SEVERELY LIMITED AT SMALL LENGTH SCALES

- At room temperature: T_H Li metal ≈ 0.68
- Li is constantly annealing. Dislocation density ↓ with time
- Small length scales: Statistically, glide can be inoperable

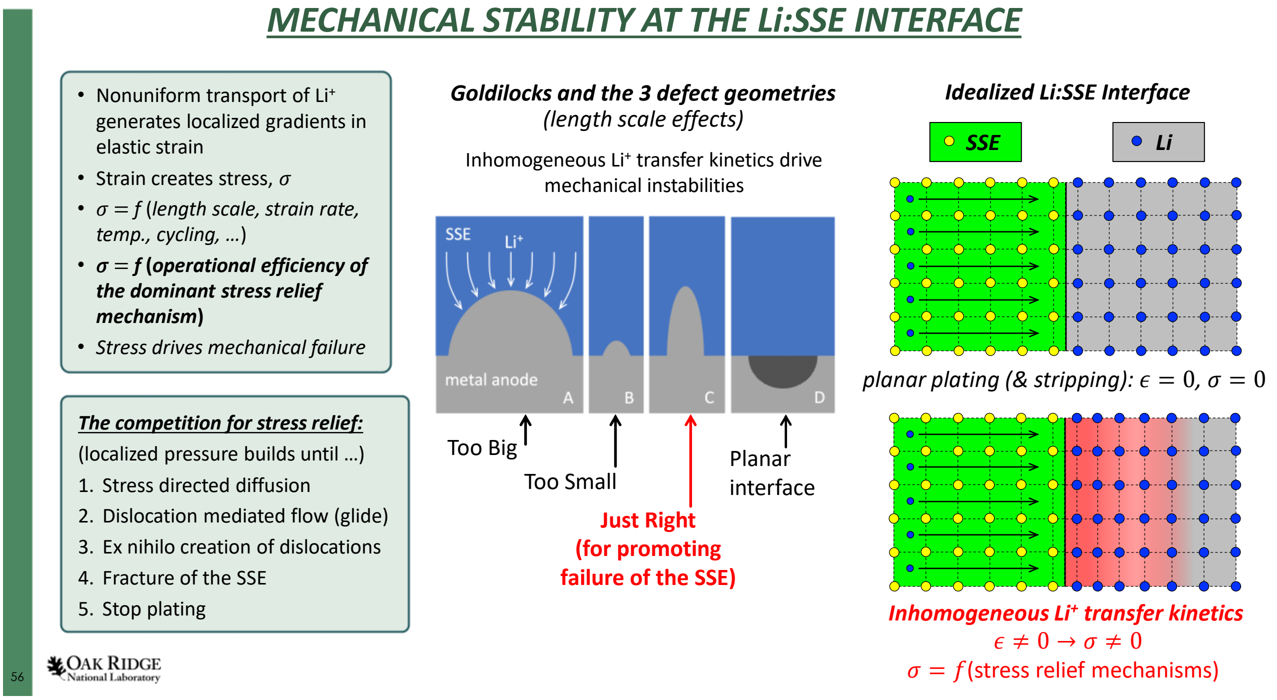
Mechanism of Action:* *Stress directed diffusion

(material transport that occurs by step-wise atomic motion)

Need point defects: ***Vacancies***

Concentration of vacancies:

- Increases exponentially with temperature
- Increases with an increase in interface area and grain boundary area



MECHANICAL STABILITY AT THE Li:SSE INTERFACE

- Nonuniform transport of Li^+ generates localized gradients in elastic strain
- Strain creates stress, σ
- $\sigma = f$ *(length scale, strain rate, temp., cycling, …)*
- ***$\sigma = f$ (operational efficiency of the dominant stress relief mechanism)***
- *Stress drives mechanical failure*

The competition for stress relief:

(localized pressure builds until …)

1. Stress directed diffusion
2. Dislocation mediated flow (glide)
3. Ex nihilo creation of dislocations
4. Fracture of the SSE
5. Stop plating

Goldilocks and the 3 defect geometries
(length scale effects)

Inhomogeneous Li^+ transfer kinetics drive mechanical instabilities

Too Big

Too Small

Just Right (for promoting failure of the SSE)

Planar interface

Idealized Li:SSE Interface

planar plating (& stripping): $\epsilon = 0, \sigma = 0$

Inhomogeneous Li^+ transfer kinetics

$\epsilon \neq 0 \rightarrow \sigma \neq 0$

$\sigma = f$(stress relief mechanisms)

ENGINEERING MECHANICALLY STABILE INTERFACES

The Mechanical Behavior of Lithium Metal

- At 'small' length scales, Li can support > 100X its bulk yield strength BECAUSE shear driven glide is severely limited – it becomes a statistical mechanics problem: probability of finding dislocations
- $\sigma = f$ (*length scale, strain rate, temp., cycling, …*)
- $\sigma = f$ (*operational efficiency of the dominant stress relief mechanisms*)

Next generation SSB materials (metallic anodes & SSEs)

★ ***Control the competition for stress relief: Eliminate fracture of the SSE***

- Engineer structure-property-processing relationships to provide efficient stress relief mechanisms operating at battery relevant length scales, strain rates, and temperatures

  Metallic Anodes:

  ★ Surface coatings or treatments

  ★ Alloying

  ★ Microscale ductility
- Modeling that captures the dominant material physics

Batteries for

Grid-Scale Energy Storage

Nian Liu

Assistant Professor

School of Chemical and Biomolecular Engineering

Georgia Institute of Technology

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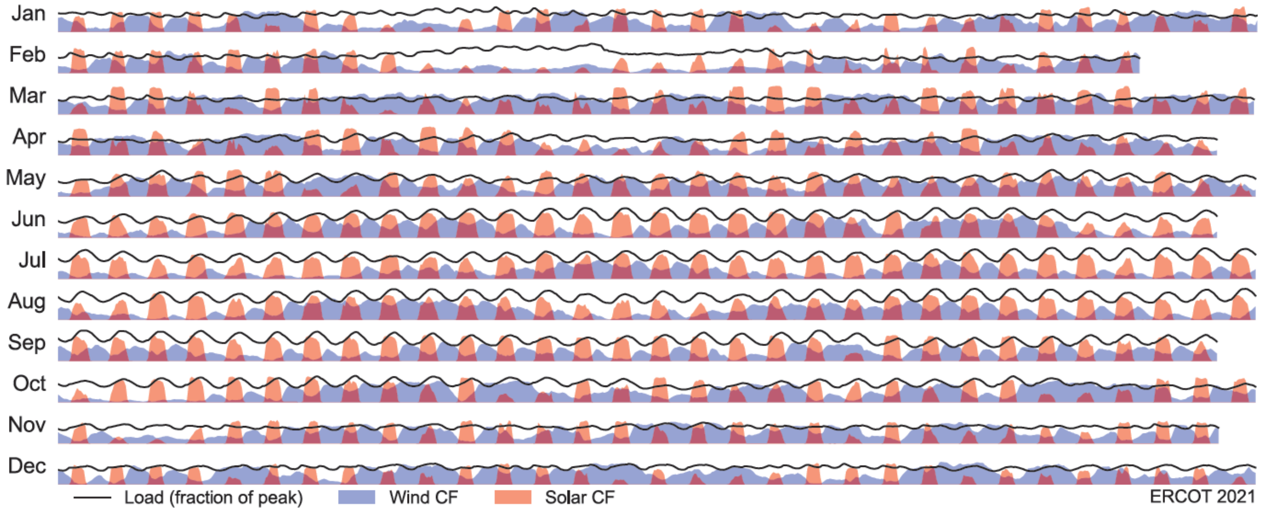
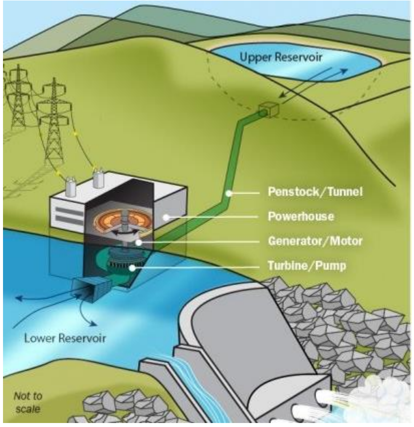
Fluctuation of renewable power supply over multiple days



Daily variability of wind (blue) and solar (red) resources in Texas relative to load (black line) in 2021. Days of the month are in the columns and months of the year are in rows. CF = Capacity factor. Source: Electric Reliability Council of Texas (2021).



Pumped Hydro Energy Storage: geographical limitation & environmental impact

Gravity Energy Storage: specific energy 10 Wh/kg

Battery Energy Storage

Hydrogen Energy Storage: roundtrip energy efficiency 40%

Grand challenge and enormous opportunity of grid-scale energy storage

- Very low cost ($10-20/kWh)
- Very long life (30 years)
- Safety
- Low maintenance

Existing Li-ion batteries production capability:
3 TWh/year (mainly for use in EVs)

To achieve 80% renewable energy,
we need 3 days of storage capacity.

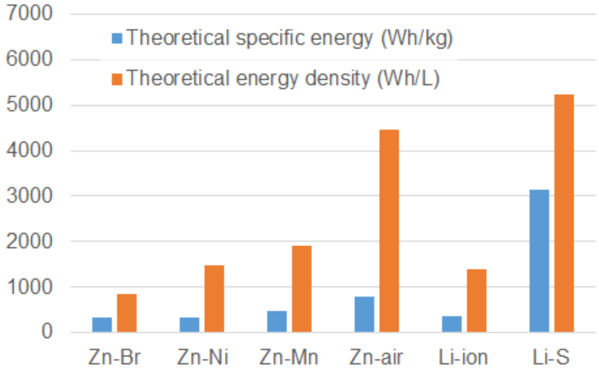
Joule, 4 (1), 21-32 (2020)

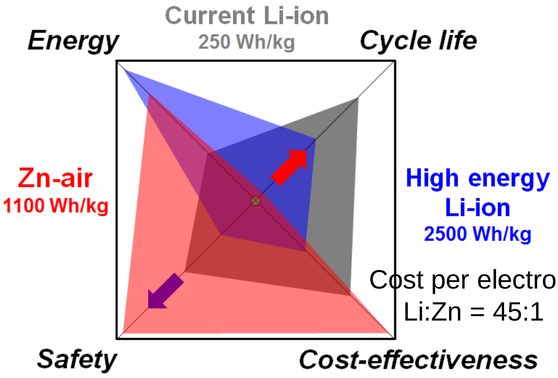
World energy consumption: 70 TWh/day
We need to install **200 TWh** storage capacity

Paris agreement: carbon neutral by 2050
Need to install at a speed of **8 TWh/year**

Intrinsic flammability of Li-ion & opportunity of Zn-based aqueous batteries

Tesla megapack (Australia)

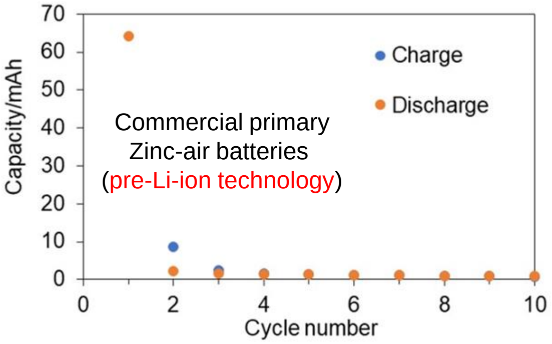


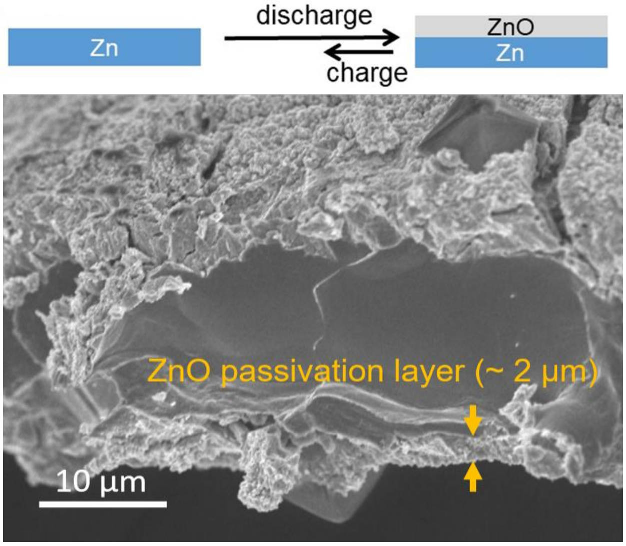


Cost per electron:
Li:Zn = 45:1

Non-rechargeable
(primary)
Zn-air battery

Irreversibility of Zn anode in alkaline electrolyte



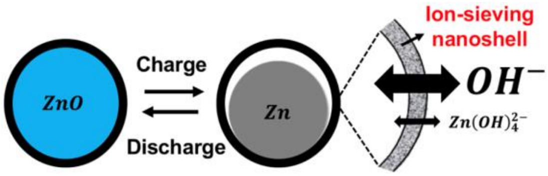


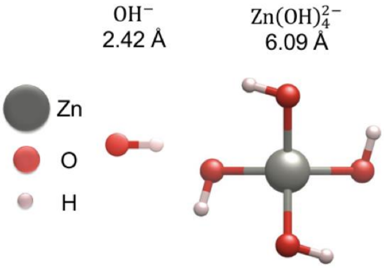
- Cannot deeply discharge (low utilization)
- Cannot recharge (poor reversibility)

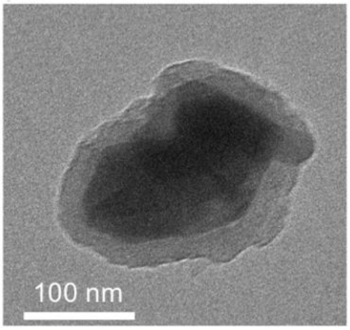
$$ZnO + H_2O + 2OH^- \leftrightarrow Zn(OH)_4^{2-}$$
$$Zn(OH)_4^{2-} + 2e^- \leftrightarrow Zn + 4OH^-$$

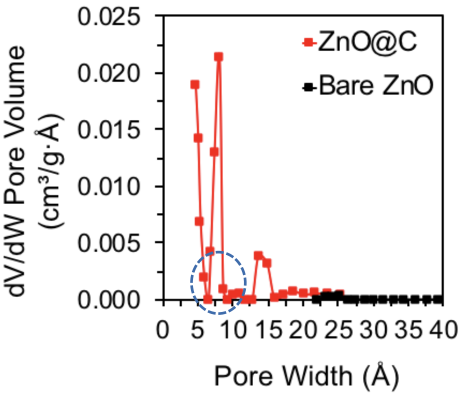
Z.-H. Wu, Y. Zhang, N. Liu*, ***Mater. Today Nano*** 6, 100032 (2019)

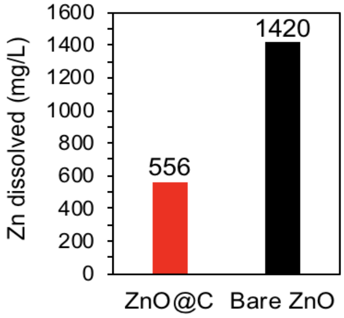
Particle-based anode material: ZnO @ ion-sieving carbon





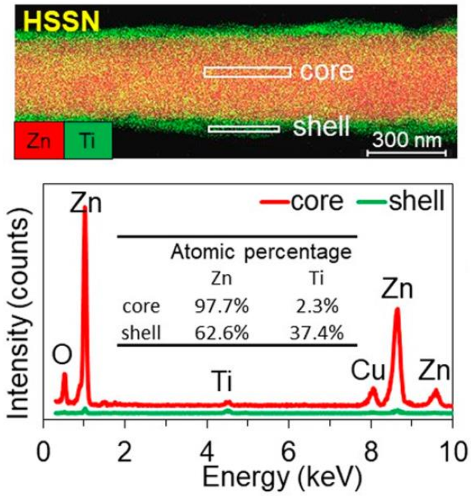




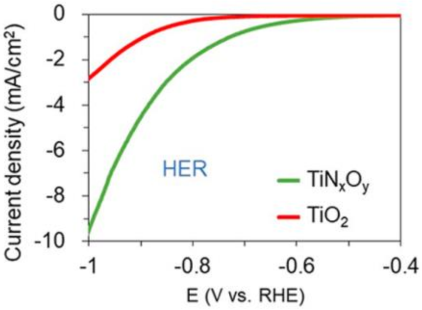


Y. Wu, N. Liu*, et al. ***Adv. Energy Mater.*** 8 (36), 1802470 (2018)

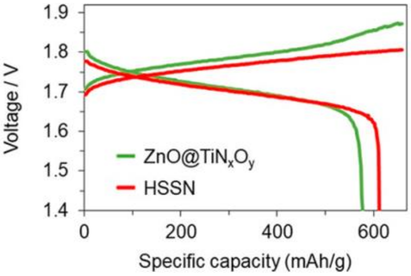
HER-suppressing sealed nanosized (HSSN) zinc anode



	Zn	Ti
	Atomic percentage	
core	97.7%	2.3%
shell	62.6%	37.4%



TiO_2 coating has low HER activity

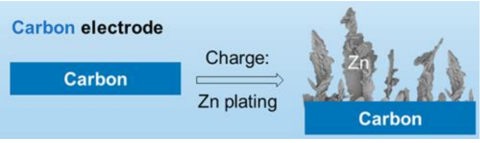


Improved Coulombic efficiency

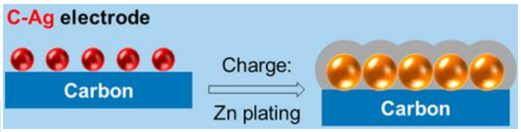
85.0% → 93.5%

Y. Zhang, N. Liu* et al. ***Nano Lett.*** 20 (6), 4700–4707 (2020)

Soluble zincate: Passive encapsulation → Active management

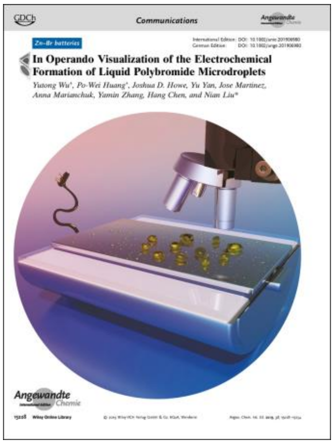


Y. Zhang, N. Liu* et al.
ACS Energy Lett.
2021, 6 (2), 404–412



Carbon fiber paper:

- Dendritic Zn deposition
- Dead Zn left behind results in capacity decay



In Operando Visualization of the Electrochemical Formation of Liquid Polybromide Microdroplets

Yutong Wu, Po-Wei Huang, Joshua D. Howe, Yu Yan, Jose Martinez, Anna Marianchuk, Yamin Zhang, Hang Chen, and Nian Liu*

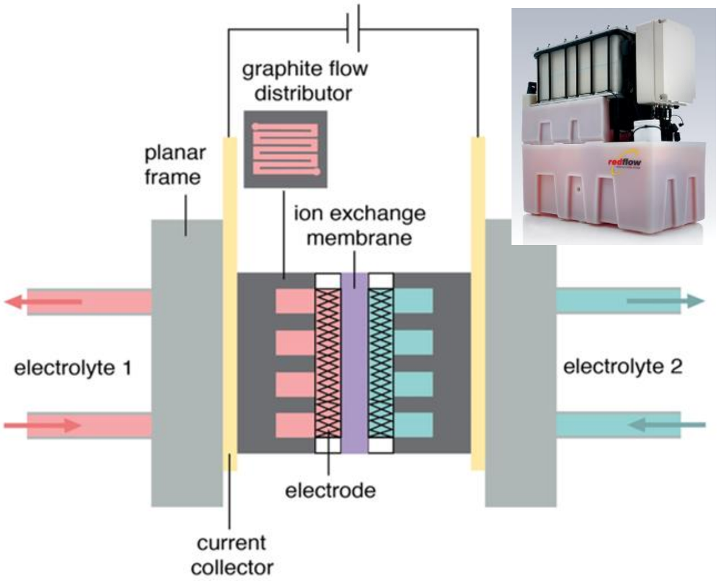
In operando Optical Microscopy for Visualizing Battery Local Dynamics

Angew. Chem. Int. Ed. 131 (43), 15372-15378 (2019)

Proc. Natl. Acad. Sci. U.S.A 116 (3), 765-770 (2019)

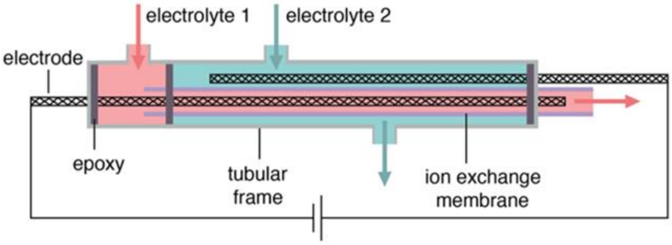
Nature Communications 11, 606 (2020)

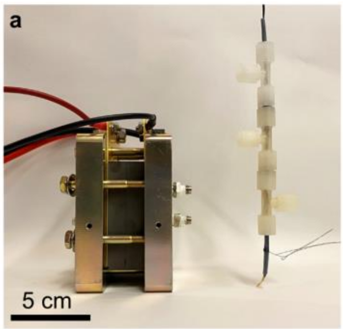
Flow batteries have decoupled power and energy
Volumetric power density of the power module

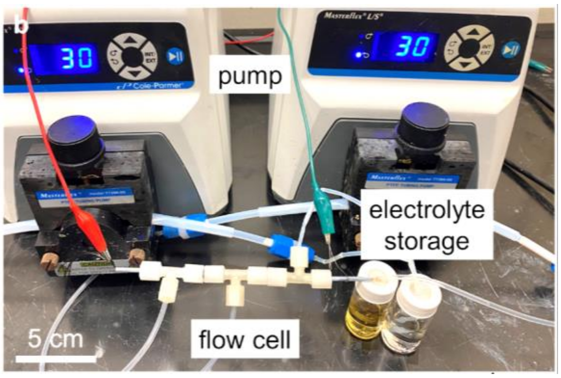


- Power density of power module ↑ (not of the electrolyte)
  Footprint and cost of power module ↓
- Planar ion-exchange membrane:
  Rate of ion transfer sometimes cannot catch up with the rate of electron transfer
  Thinner membrane is easier to break
- Inactive parts of the power module: additional volume, weight and cost
  Bipolar plates and frames need certain thickness for rigidity
  Flow channels need certain thickness and width for reliable machining

A microtubular flow battery cell



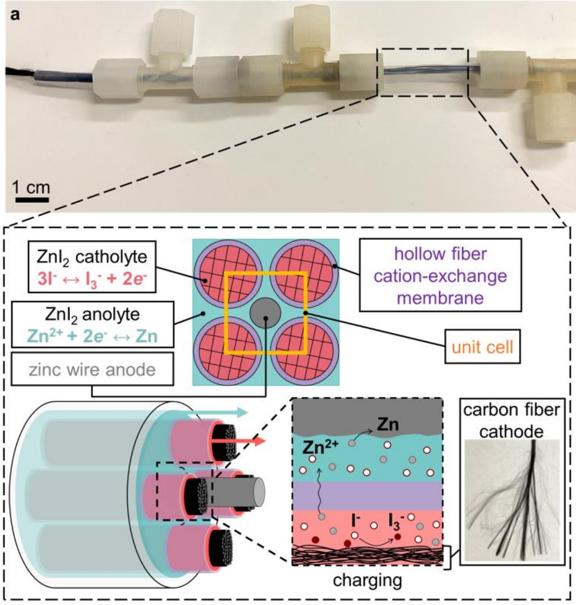




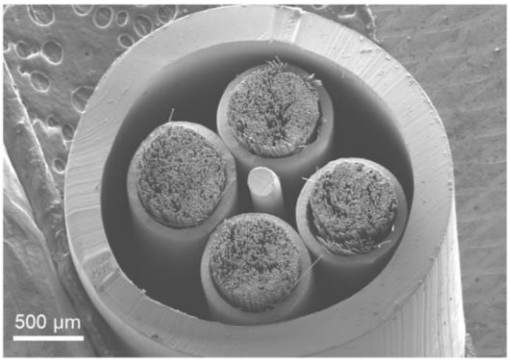
- ✓ Distance between electrodes is smaller
- ✓ Membrane surface area is bigger in a given volume
- ✓ Microtubular membrane serves as the flow distributor, and eliminates inactive parts (higher vol. power density, lower cost)
- ✓ Modular design, easy to scale up

Y. Wu, F. Zhang, T. Wang, X. Xie*, R. P. Lively*, N. Liu* et al.
Proc. Natl. Acad. Sci. U.S.A. 2023, 120 (2), e2213528120

A microtubular Zn-I_2 flow cell with a bundle of four microtubes

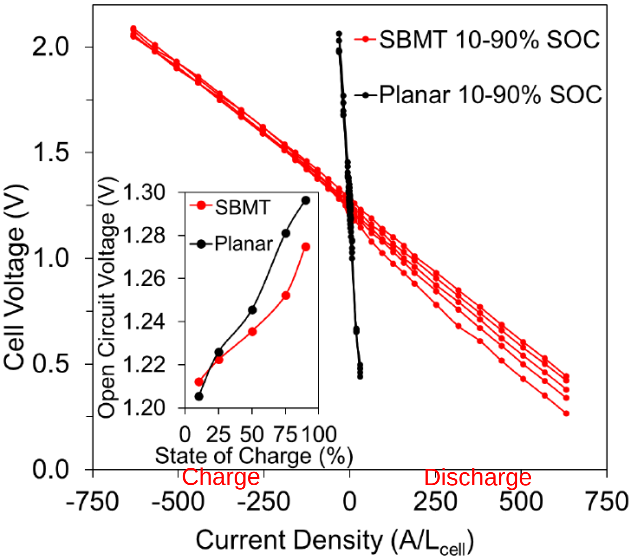


Nafion microtube
(hollow fiber)
from Perma Pure
Outer diameter: 600 μm
Wall thickness: 75 μm



Y. Wu, F. Zhang, T. Wang, X. Xie*, R. P. Lively*, N. Liu* et al. ***Proc. Natl. Acad. Sci. U.S.A.*** 2023, 120 (2), e2213528120

SBMT power module sustains ultra-high current density



SBMT: sub-millimeter, bundled microtubular

A poly(vinylidene fluoride) (PVDF) microtubular membrane module with ~ **1,300** hollow fibers inside (the size of the Swagelok is 1 inch).

Y. Wu, F. Zhang, T. Wang, X. Xie*, R. P. Lively*, N. Liu* et al.
Proc. Natl. Acad. Sci. U.S.A. 2023, 120 (2), e2213528120

Summary and Acknowledgement

- Batteries for grid-scale storage
- Zinc-based batteries
- Flow batteries


Dec 2023 Group Lunch

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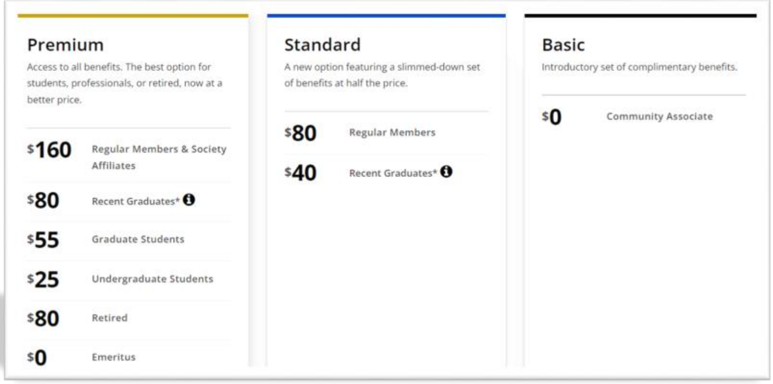

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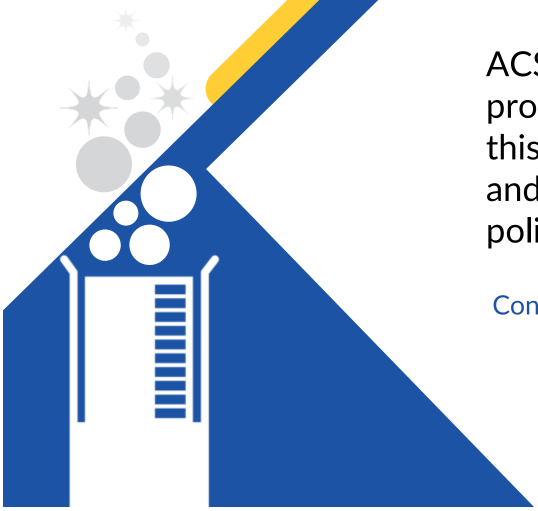

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