

# Next-Generation Batteries for Electric Transportation and Stationary Storage

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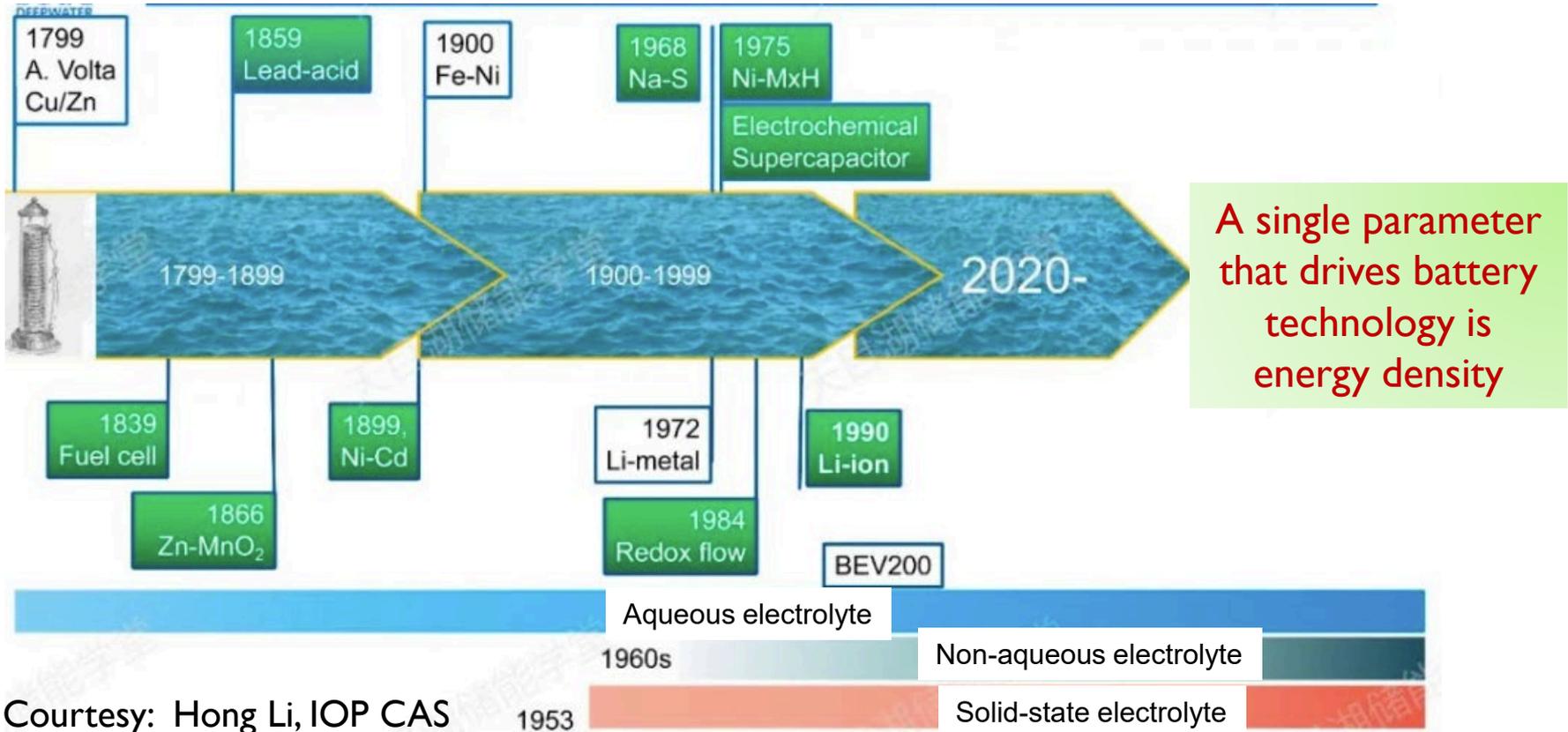
 @YanYao2

UNIVERSITY of  
**HOUSTON**

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CULLEN COLLEGE of ENGINEERING  
Department of Electrical & Computer Engineering

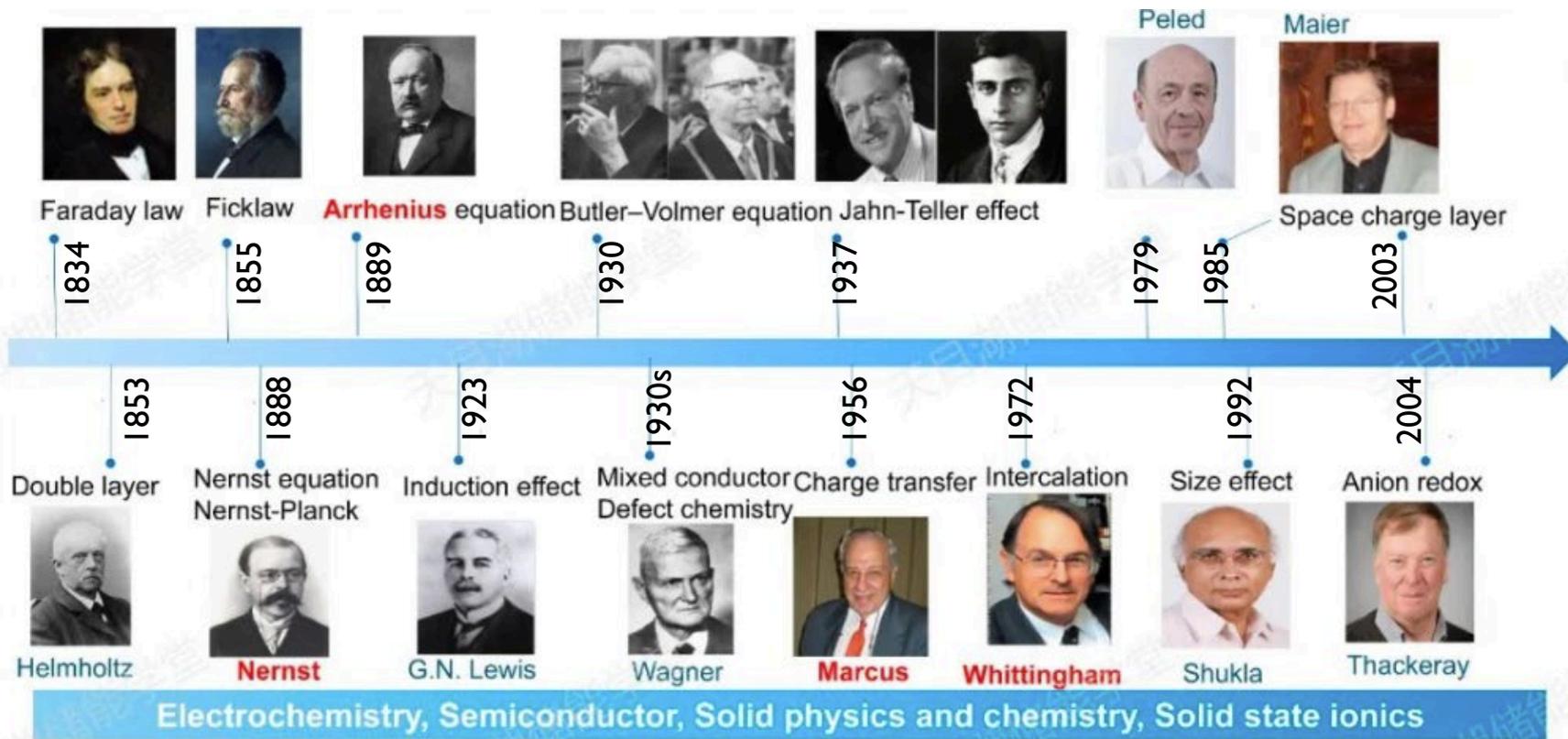
# 220 Years of Battery Research



Courtesy: Hong Li, IOP CAS

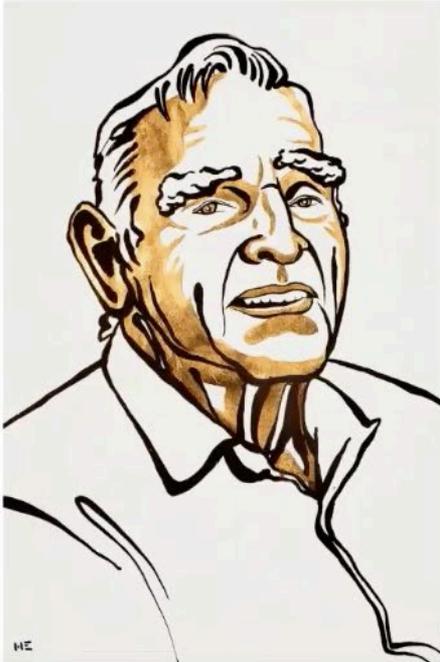
1953

# Fundamental Concepts in Battery Research



Courtesy: Hong Li, IOP CAS

# 2019 Nobel Prize in Chemistry goes to



John B. Goodenough  
Cathode materials: LCO/LMO/LFP



M. Stanley Whittingham  
Intercalation concept:  $\text{TiS}_2$



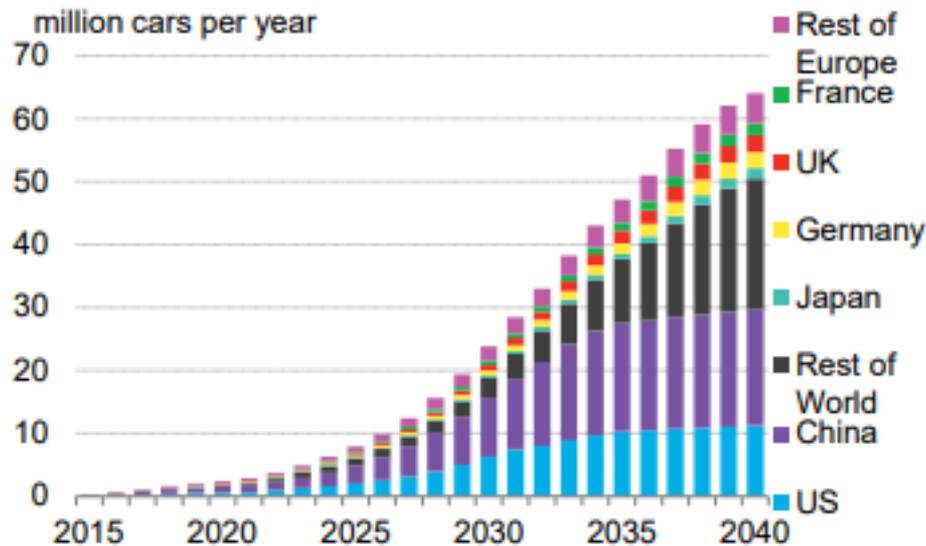
Akira Yoshino  
First prototype Li-ion batteries

*“for the development of lithium-ion batteries”*

# Need Battery Breakthrough to Enable Full Penetration of EVs

In 2019, 2% PHEV+BEV penetration

Figure 3: Annual global EV sales by market



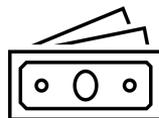
Source: Bloomberg New Energy Finance. For a detailed descriptio



High Energy  
> 300 miles range



Fast Charging  
Charge in < 15min



Cost  
< \$30K, 300 mile EVs

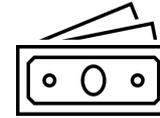
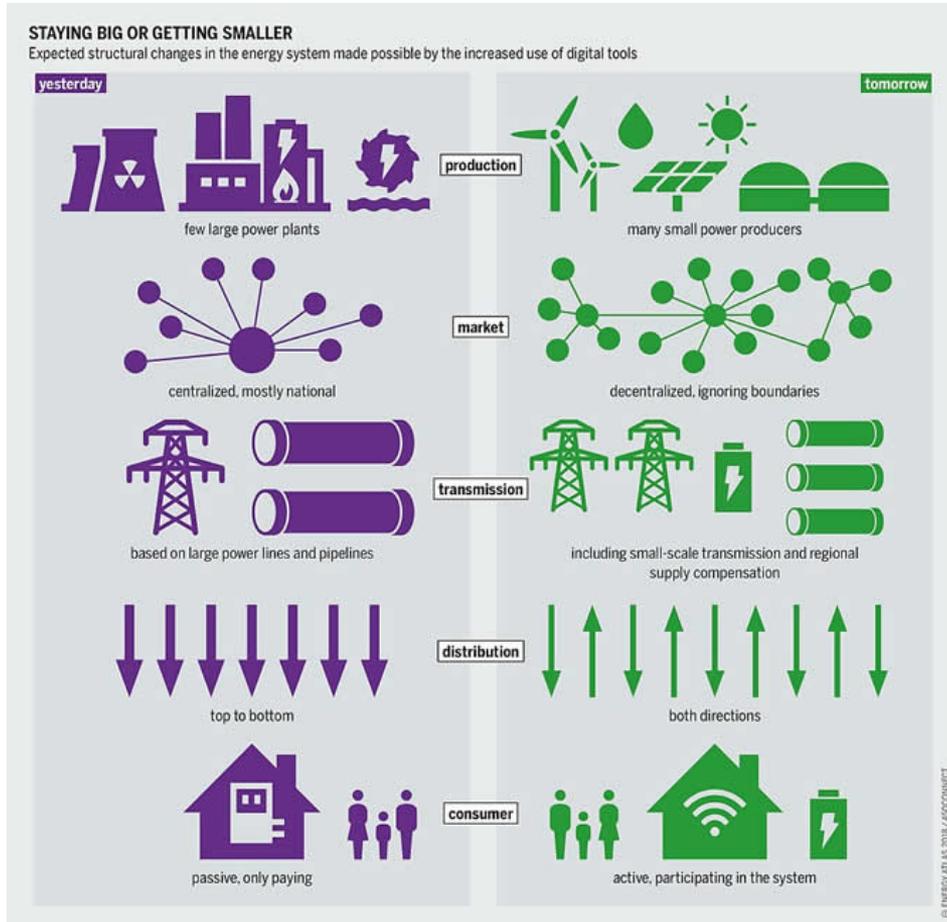


Battery Lifetime  
> 12 year, > 150k miles



Safety  
Solid, non-flammable  
electrolytes

# Need Battery Breakthrough to Enable Smart Electric Grid



Levelized Cost  
5 cents/kWh-cycle



Battery Lifetime  
5000 cycles

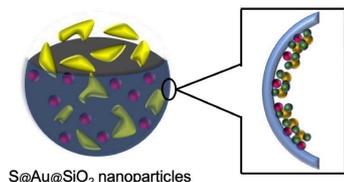


Safety  
Non-flammable  
electrolytes

# Energy Storage Program in Yao Group

## Li-ion battery

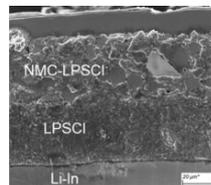
ACS AMI. ASAP (2020)  
Chem. Comm. 51,229 (2015)



S@Au@SiO<sub>2</sub> nanoparticles

## Solid-state Li battery

ACS Energy Lett. (2020)  
Joule (2020)



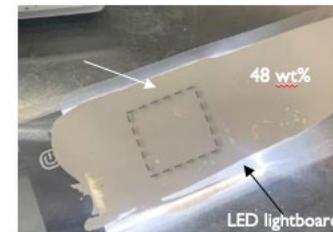
## Characterization

DOE VTO Project



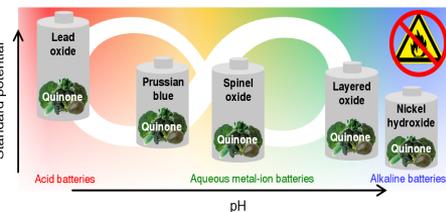
## Manufacturing

UH AMI Project



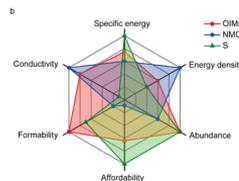
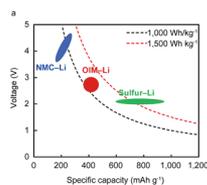
## Grid-scale storage

Nature Mater. 16, 841 (2017)



## Organic battery

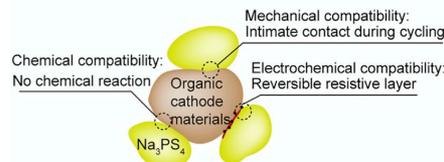
Chem Rev. 120, 6490 (2020)  
Joule 2, 1690 (2018)



## Na battery

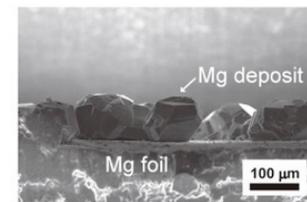
Joule 3, 1349 (2019)  
Angew Chemie 130, 2660 (2018)

Favorable electrode-electrolyte interface



## Mg battery

Nature Energy 5,1043 (2020)  
Nature Energy 5, 645 (2020)  
Nature Comm. 8, 339 (2017)



# High-energy Solid-State Organic-Lithium Batteries

# What are Solid-state Li-metal Batteries



Li-ion battery



Solid-state Li metal battery

Lithium-Metal  
Anode (-)

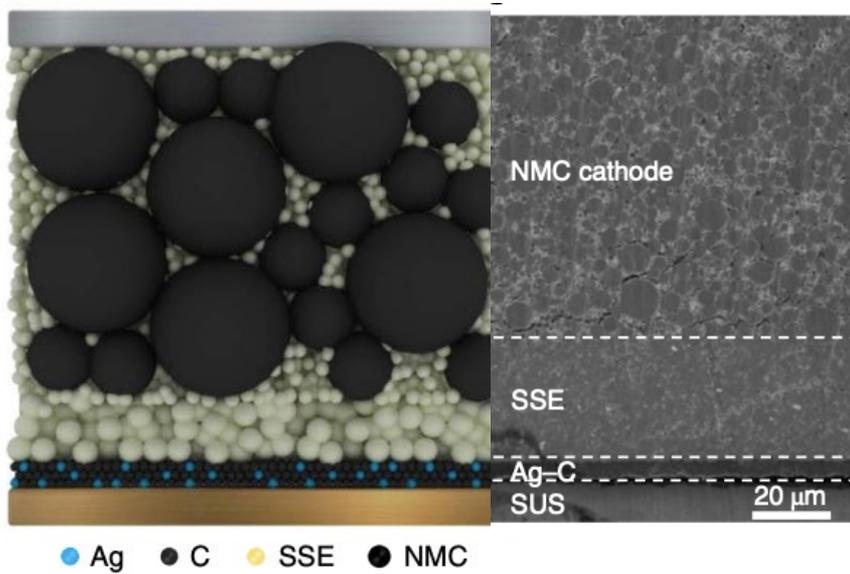
Cathode (+)

Greater range

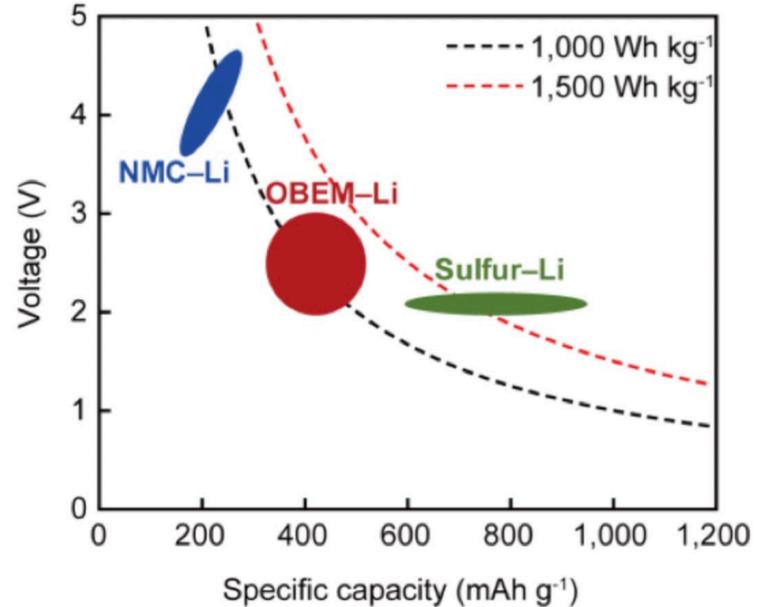
15-minute fast  
charge

Safer operation

# Motivations for Organic-Lithium Batteries

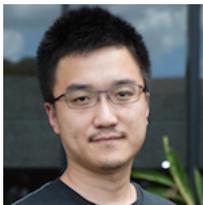


Y. G. Lee et al. Nat. Energy 2020, 5, 299

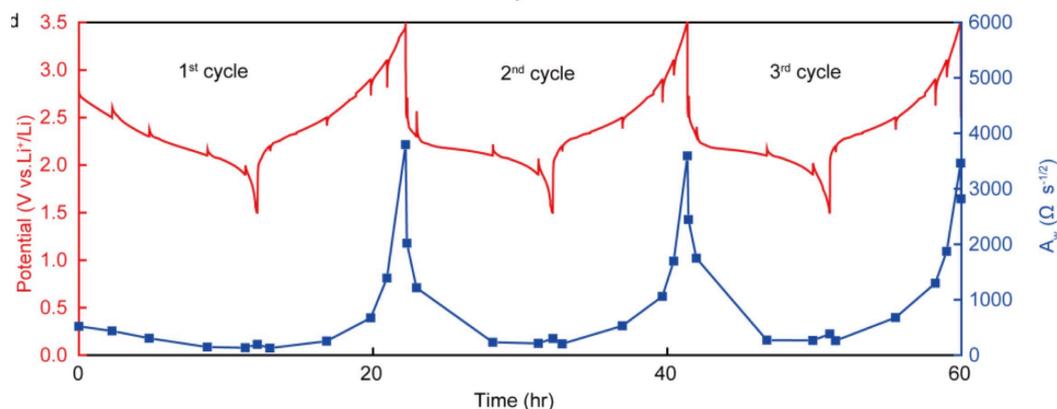
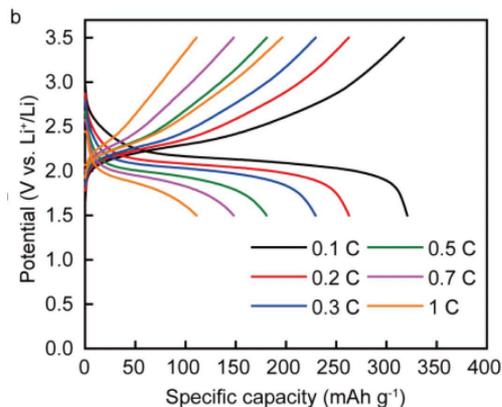
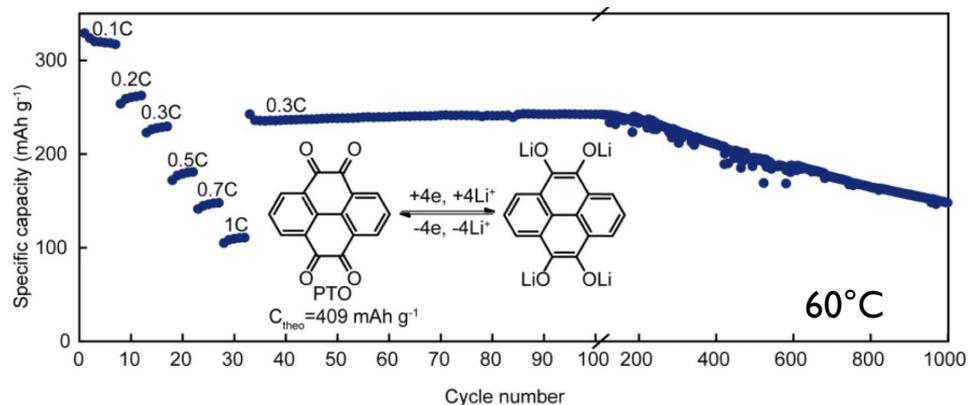
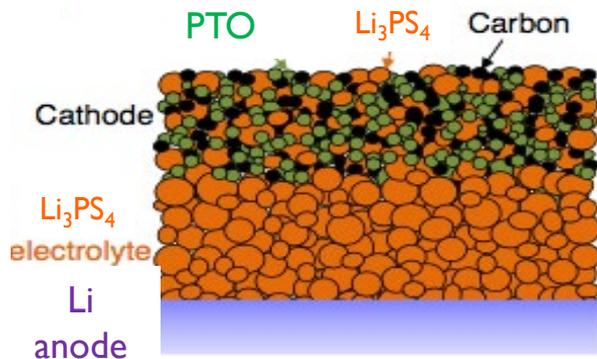


- Organic compounds with **well-understood redox-active functional groups** can reversibly store/release multiple electrons and cations per molecule.
- Organic-lithium batteries can deliver **material-level specific energies** of 1000 Wh kg<sup>-1</sup>

# An Organic-Li cell cycles for 1000 Cycles



Fang Hao  
(GM R&D)



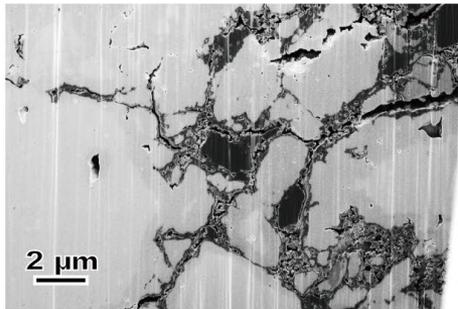
material utilization of 78%

Hao, Liang, Yao\*, ACS Energy Lett., in press

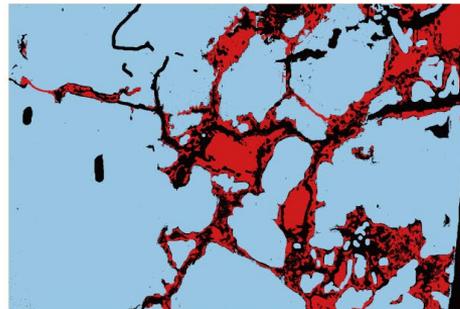
# Cryo-milled Cathode Composites

Hand-milled

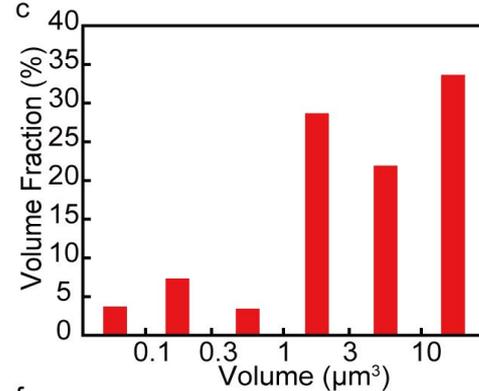
a



b

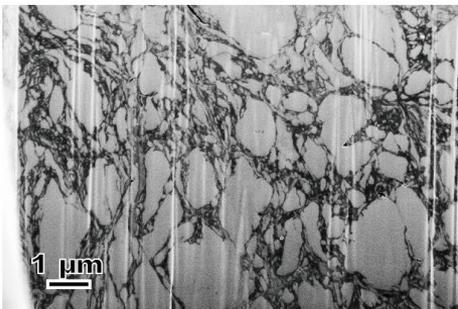


c

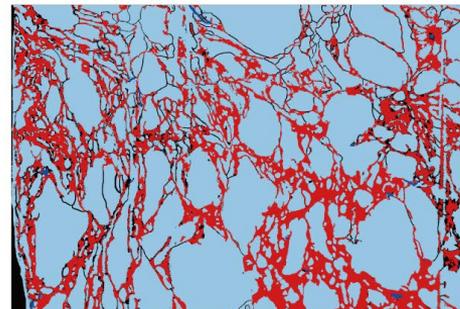


Cryo-milled

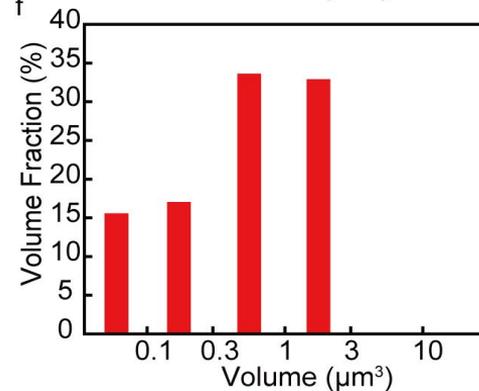
d



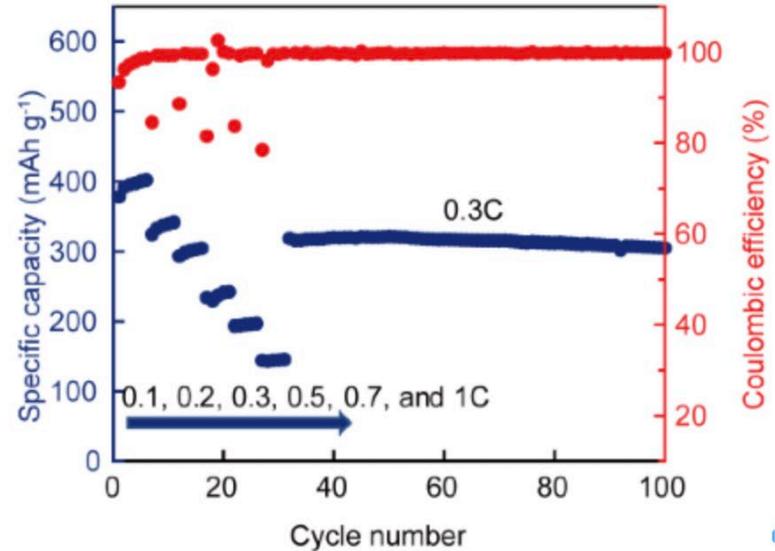
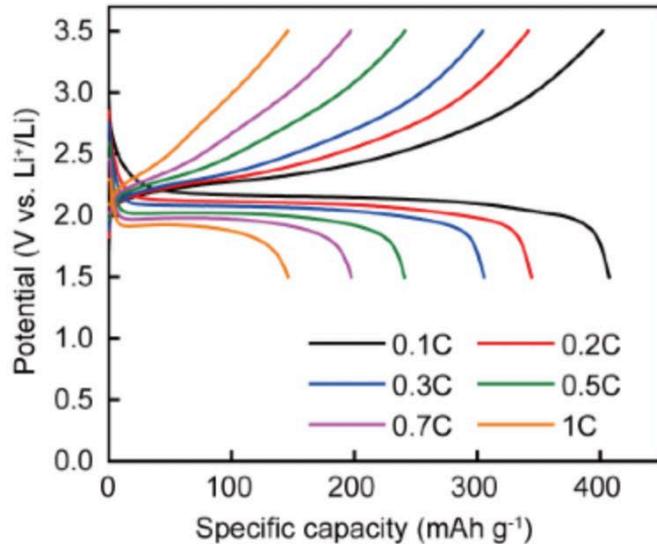
e



f



# Cryo-milled Samples show of 99.5% Material Utilization

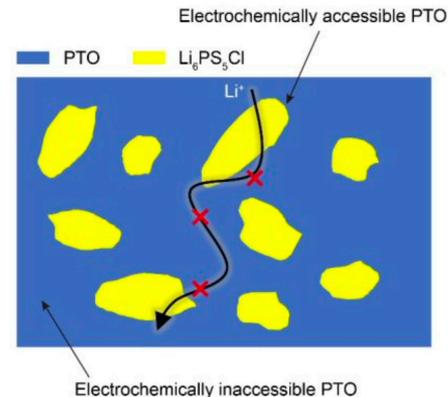
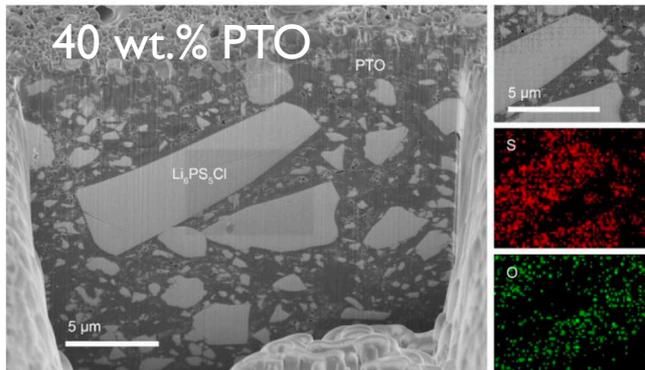
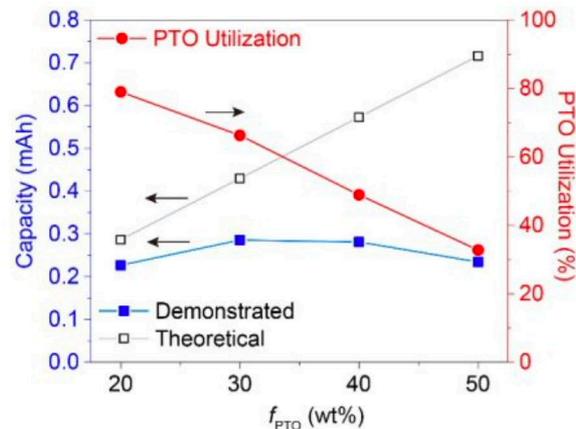
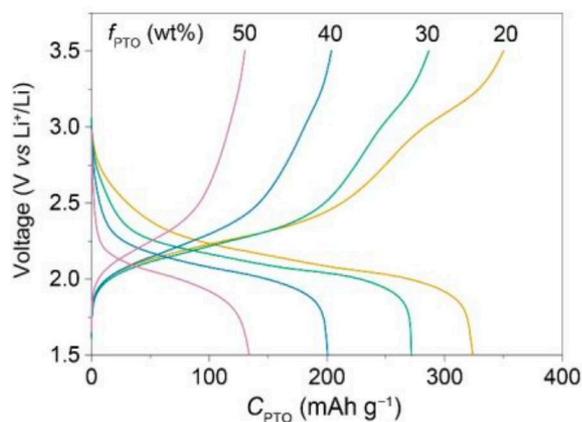


- Cryo-milled composites deliver capacities of 407 mAh g<sup>-1</sup>, a material utilization of 99.5%.
- The material-level specific energy of 828 Wh kg<sup>-1</sup> based on the weight of Li<sub>4</sub>PTO.
- The cathode only contain 20 wt% active materials.

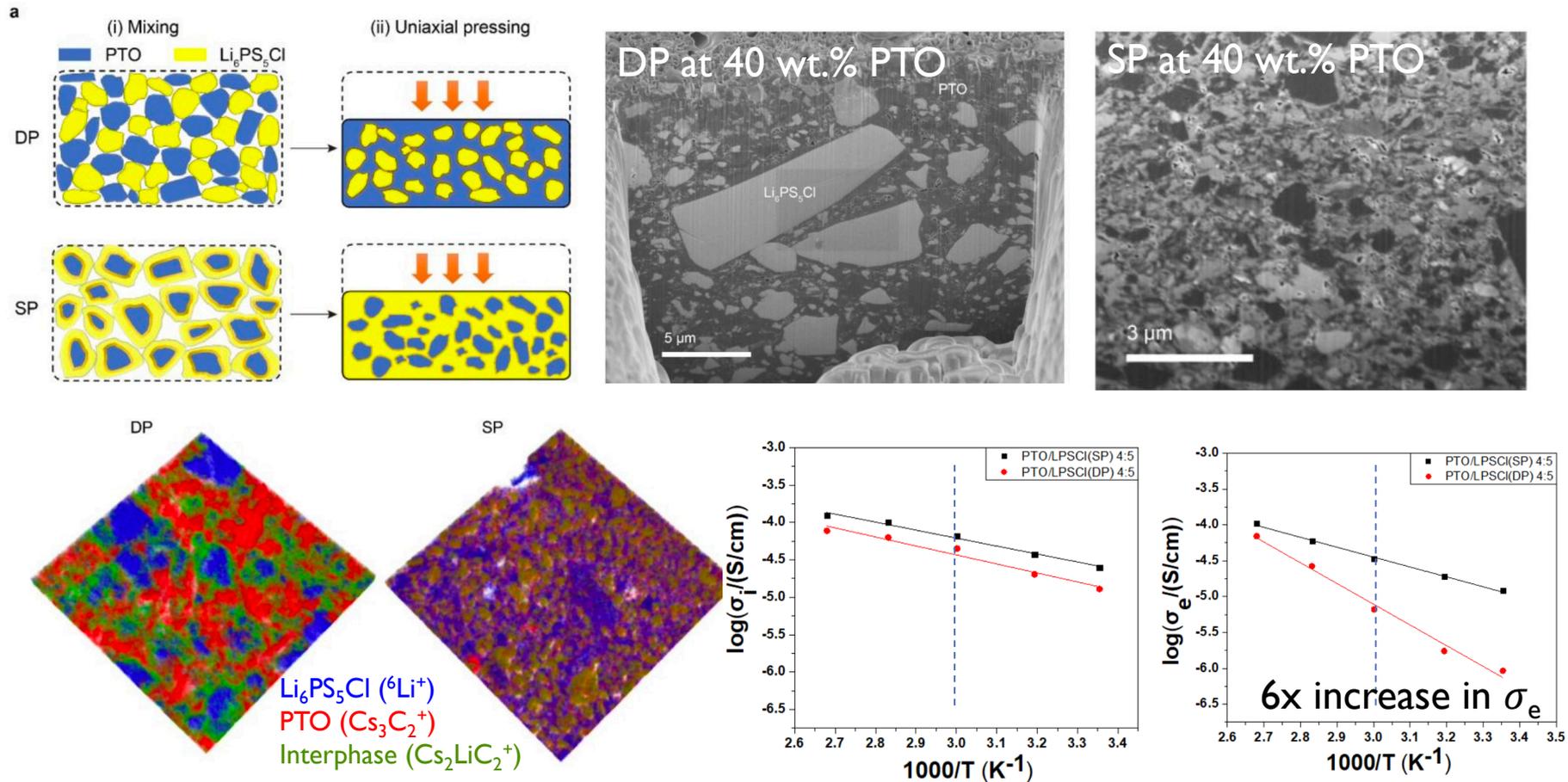
# Issues with Increasing Active Materials Fraction



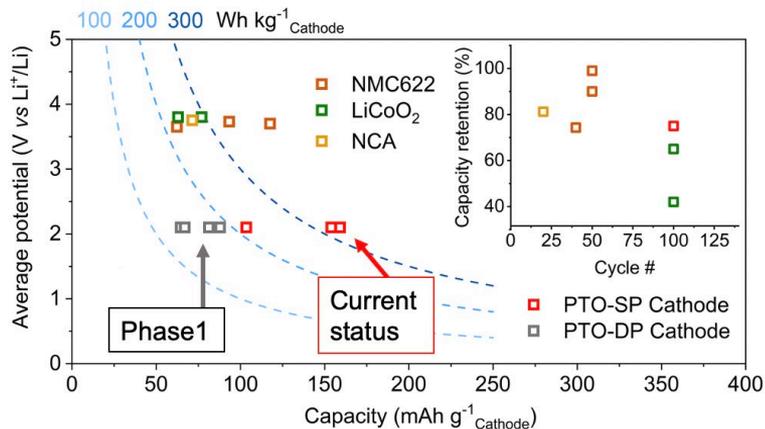
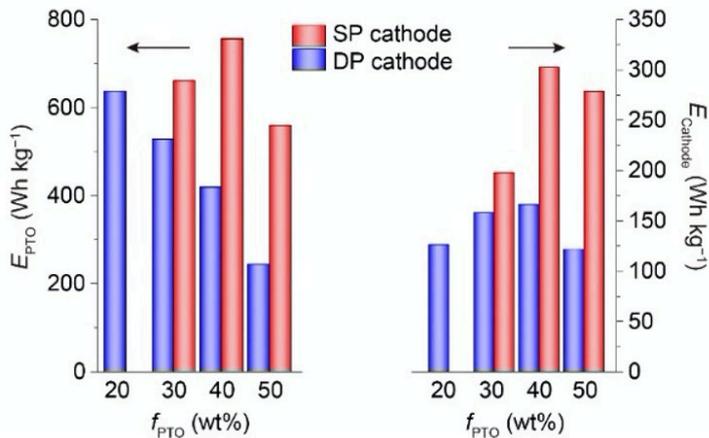
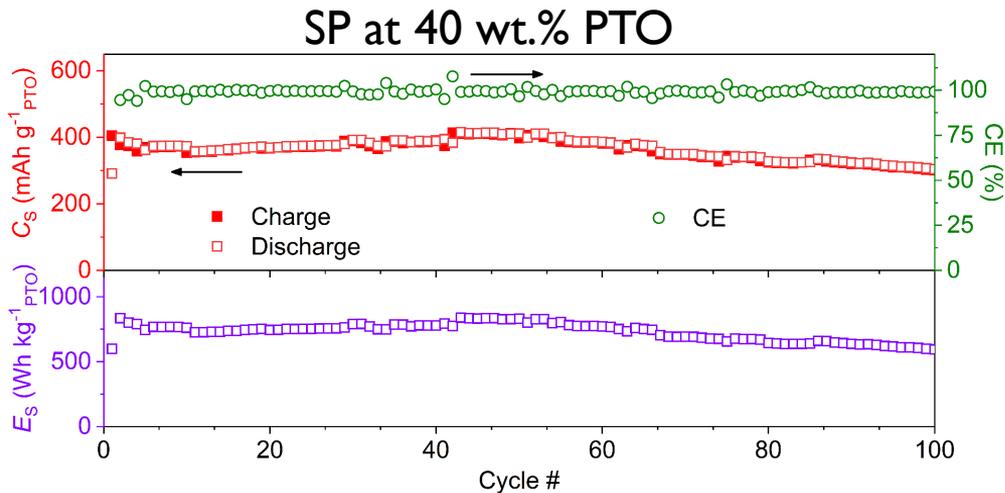
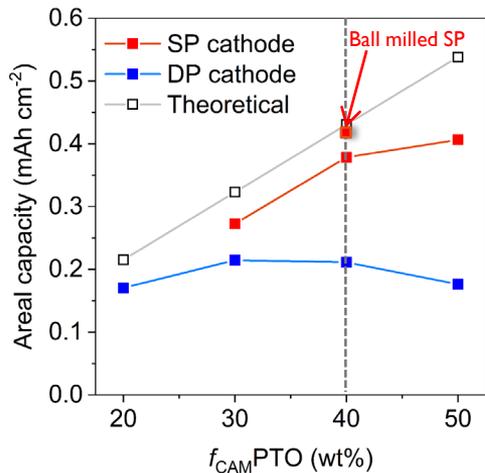
Dr. Jibo Zhang



# Solution Process for Better Microstructure



# Improved Battery Performance at Electrode-level

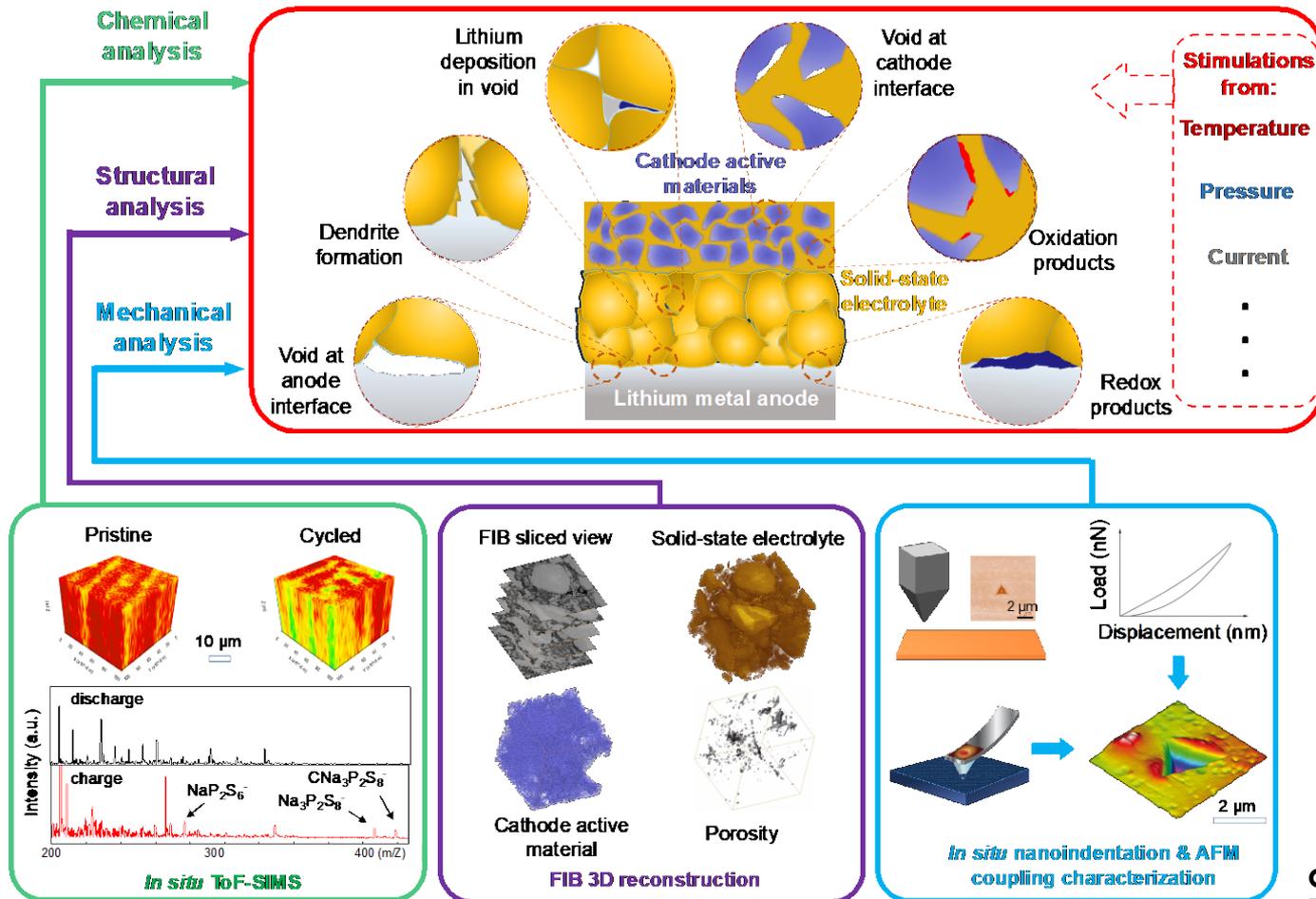


# Diagnostic Platform for Understanding Failure Mechanisms of Solid-state Li Batteries

# UH-Rice Team

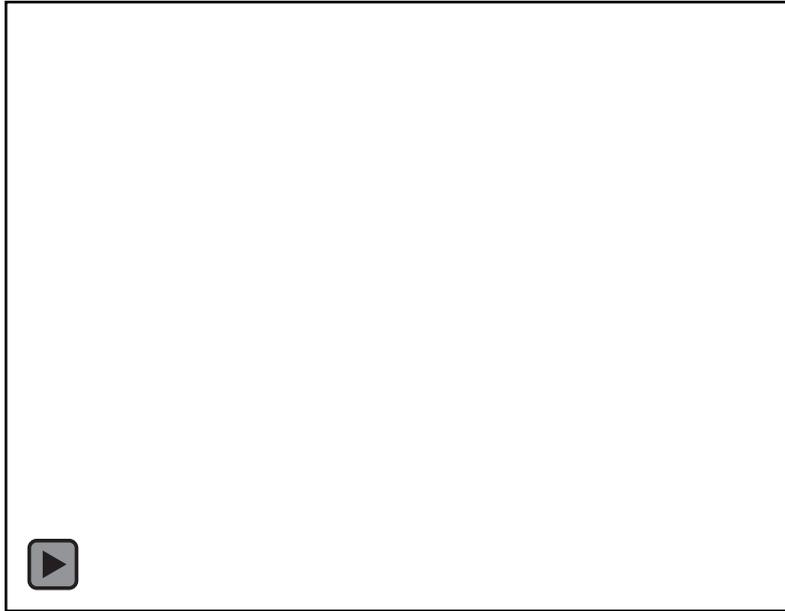


## Interfacial evolutions induced by external stimulations



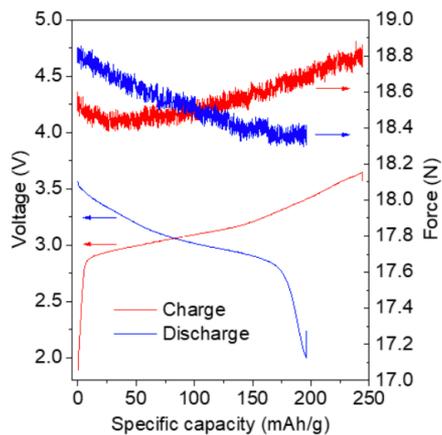
# Air-free transfer vessel with an in-situ cell test platform

SAMPLES ARE AIR-SENSITIVE

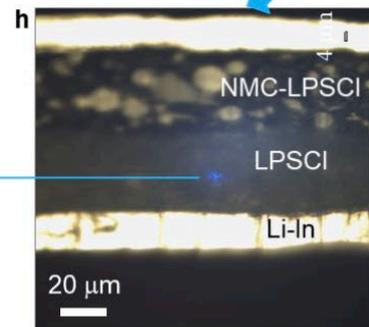
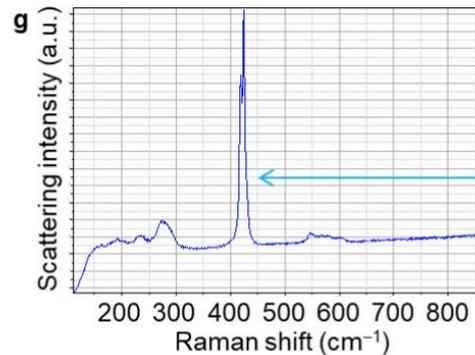
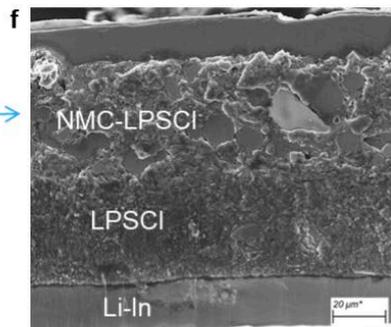
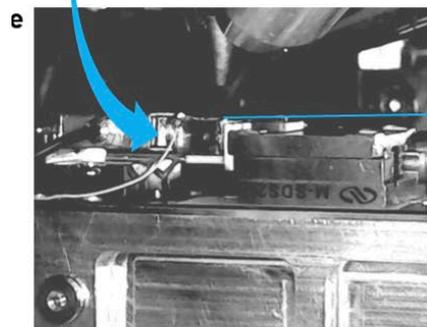
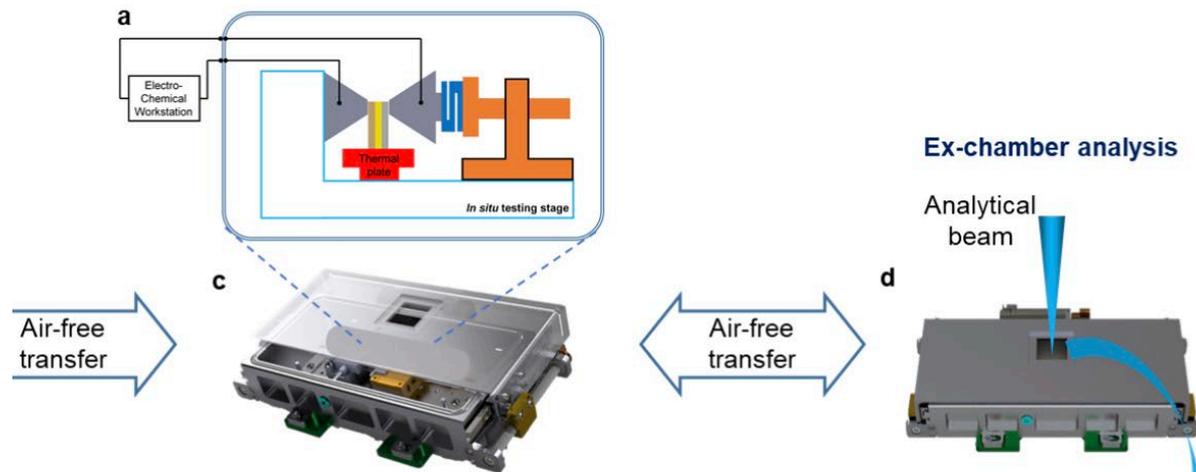


PROTOTYPE

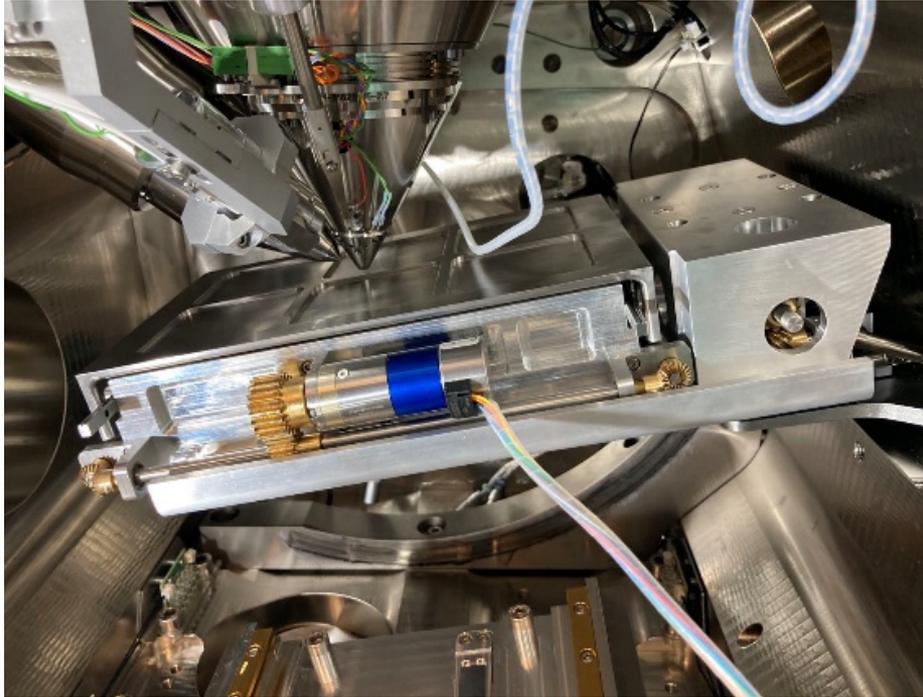




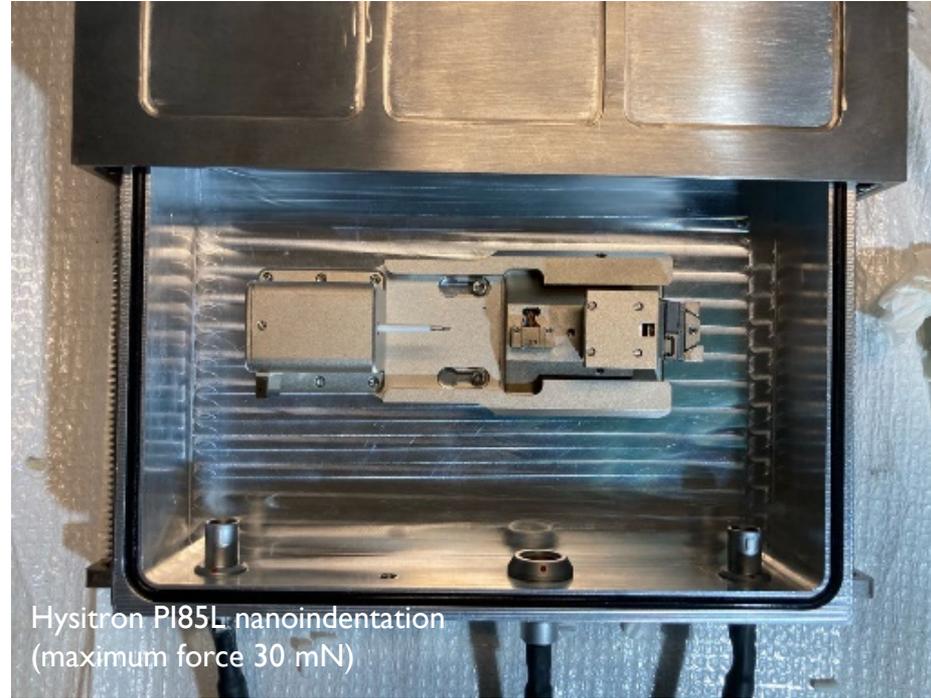
**Figure 3. Voltage profile and pressure change of an NMC/LPSCI/Li-In micro-cell tested in the transfer vessel.**



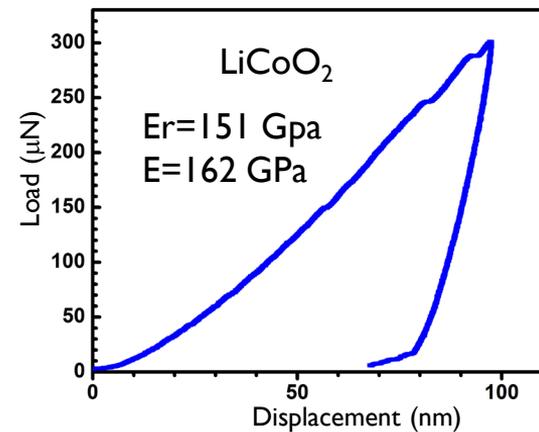
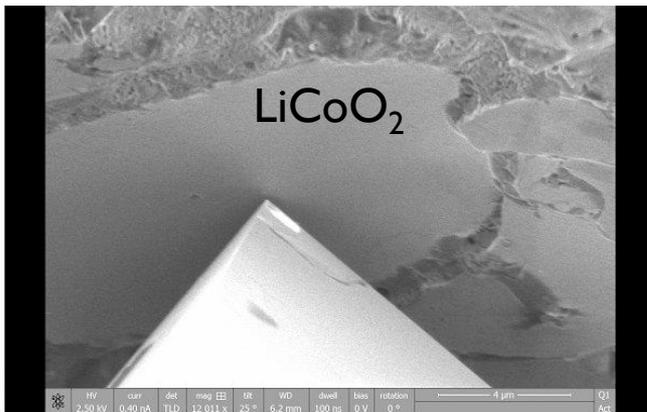
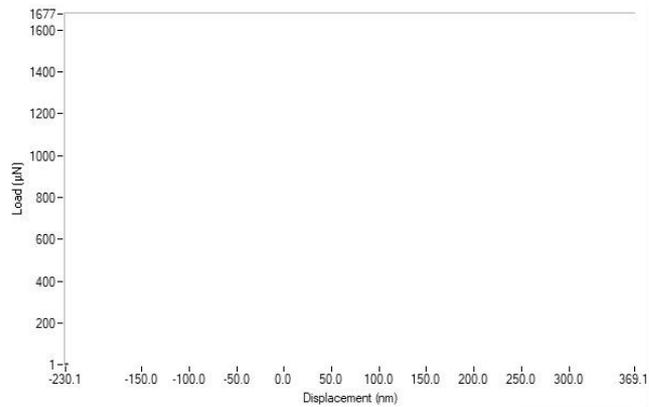
# In-SEM Nano-indentation for Air-sensitive Samples



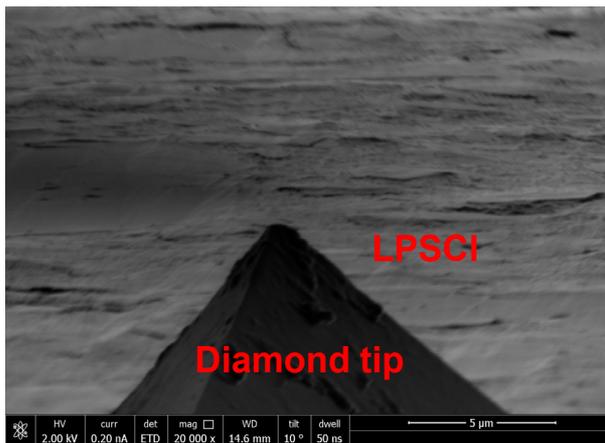
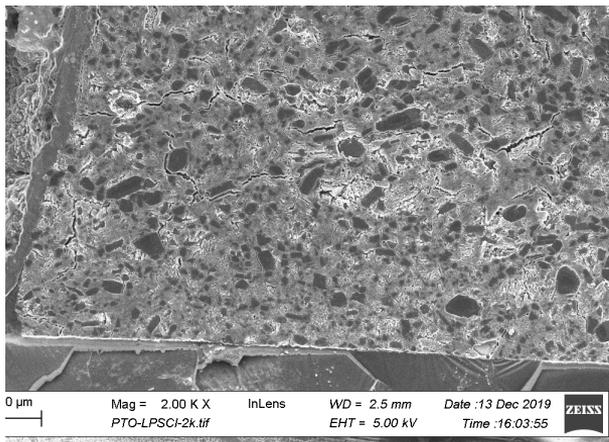
Box Inside SEM



Indenter inside box



 HYSITRON™

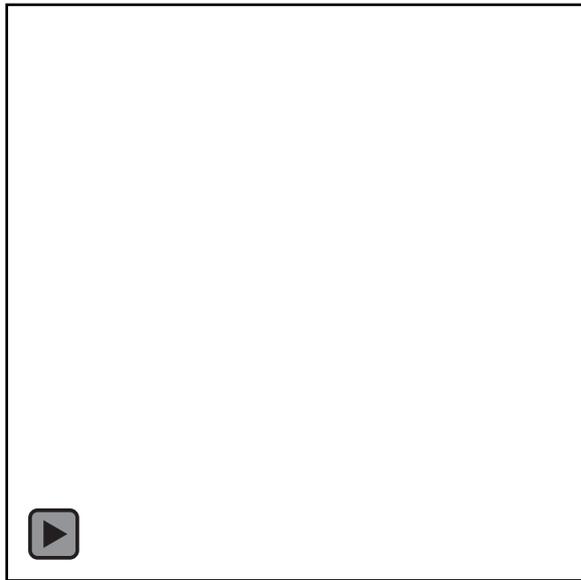


LPSCI	E (GPa)	H (GPa)
1	12.8	0.74
2	19.5	1.66
3	25.2	4.83

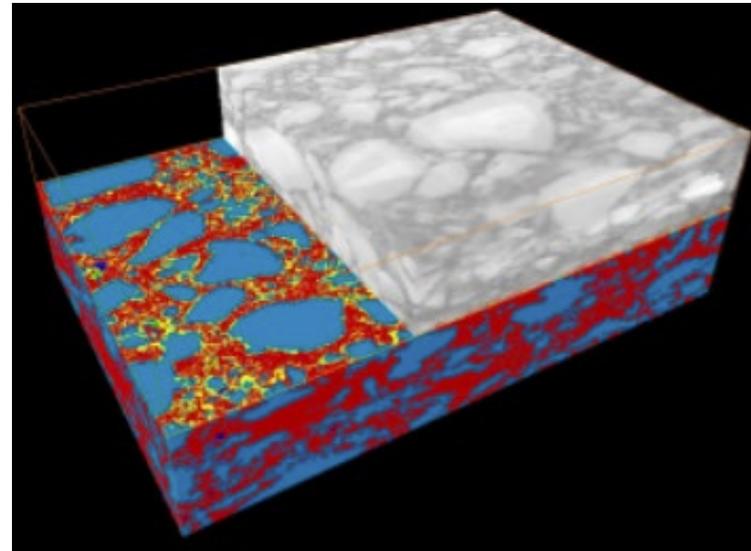
# Cathode Microstructure Analysis by Slice & View



**Helios FIB**



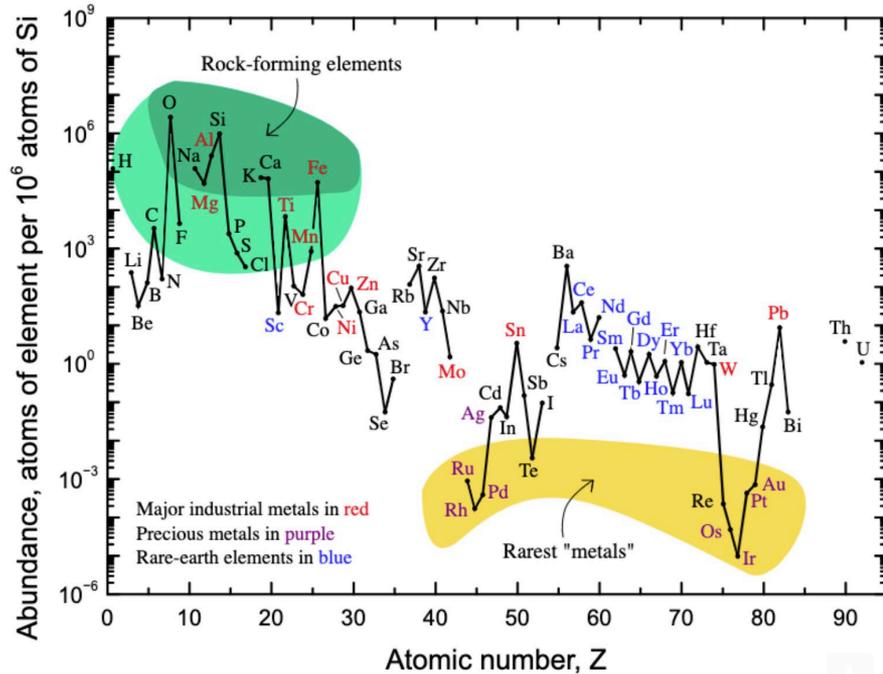
Size: 4  $\mu\text{m}$



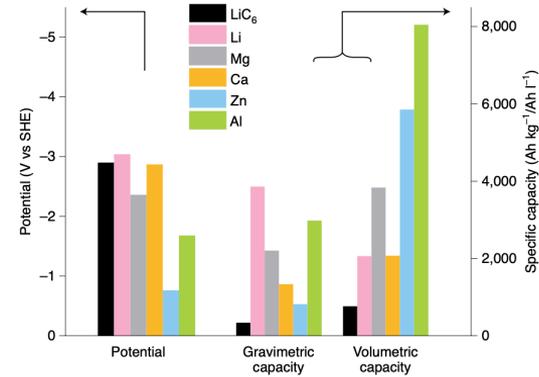
	Total Vol. ( $\mu\text{m}^3$ )	Volume Fraction
Organic/C	199	51.4%
Electrolyte	184	47.7%
Pores	3.3	0.9%

# High-Power Mg batteries for Grid-scale Energy Storage

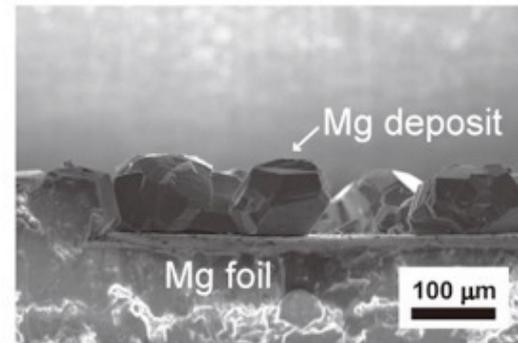
# Mg Batteries for Grid-scale Energy Storage



Top 10 most abundant elements

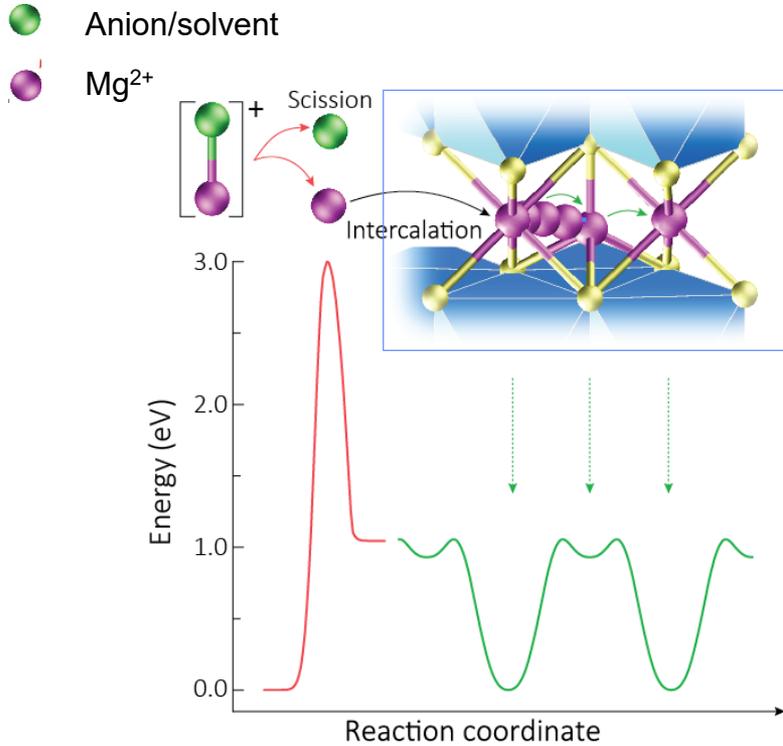


Nature Energy 5, 645 (2020)



ACSAMI 7, 7001 (2015)

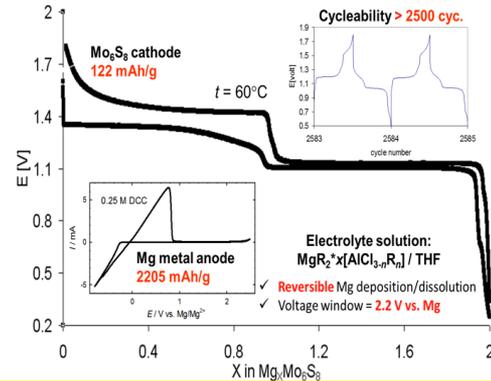
# Low Capacity and Low Power of Mg<sup>2+</sup> Cathodes



H. D. Yoo, Y. Yao, *Nat. Commun*, 2017, **8**, 339.

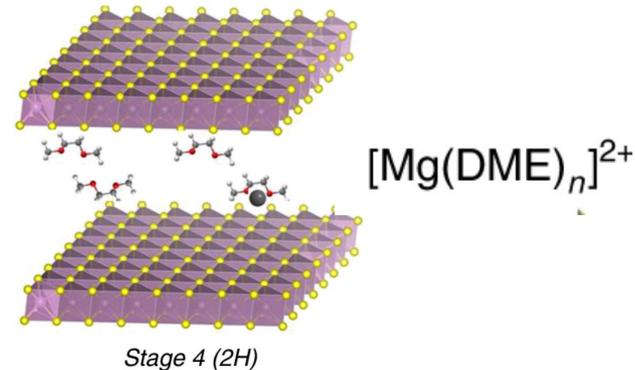
## Elevated temperatures

D. Aurbach et al., *Nature*, **407** (2000) 724.



## Storing Mg cation in its complex form

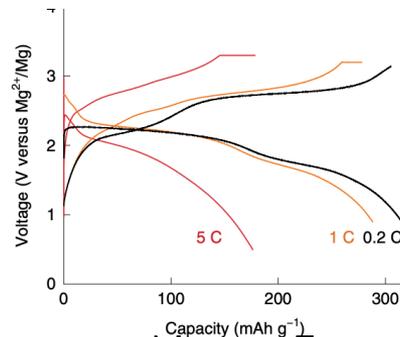
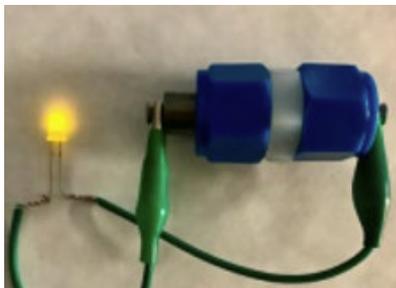
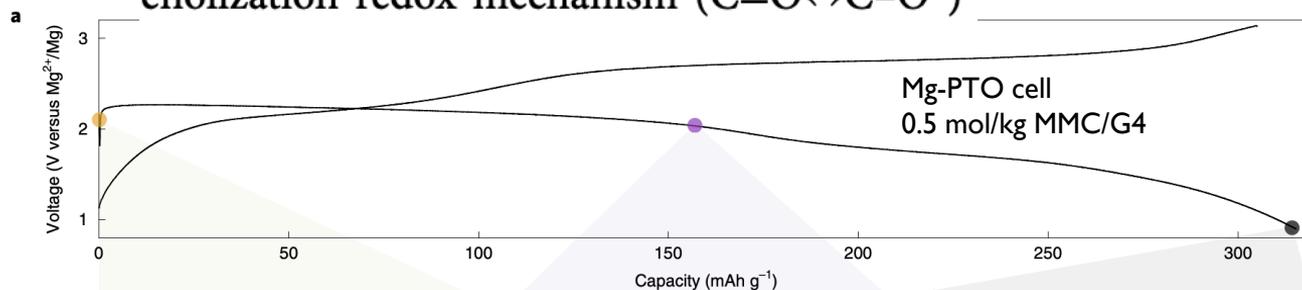
Zhao-Karger, Fichtner et al., *Nature. Comm*, 9 **5115** (2018)



# Heterogeneous Enolization Redox Cathode

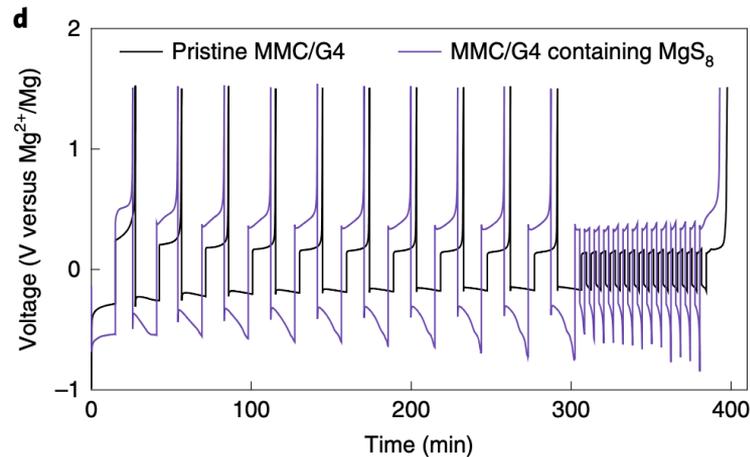
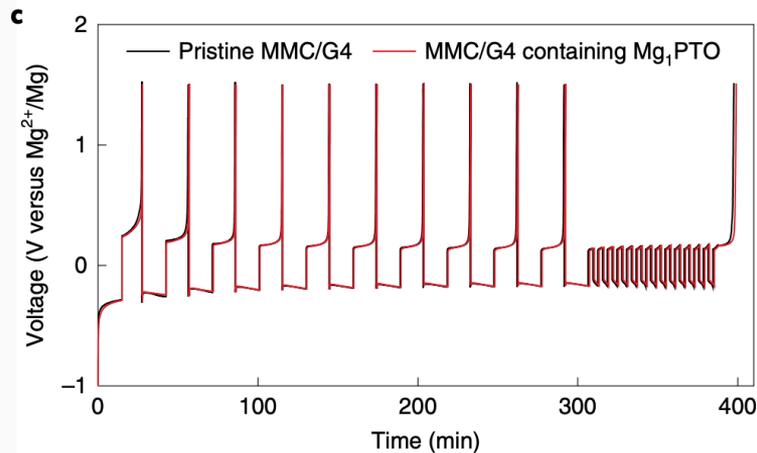
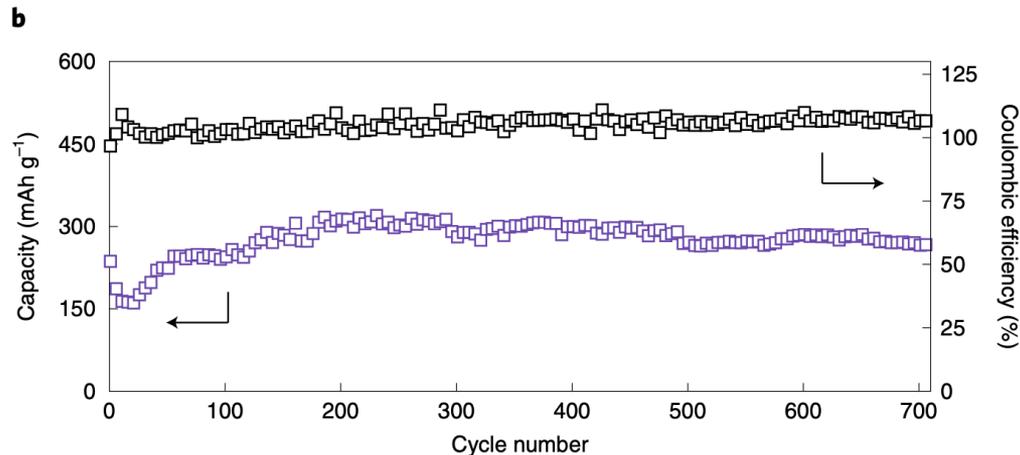
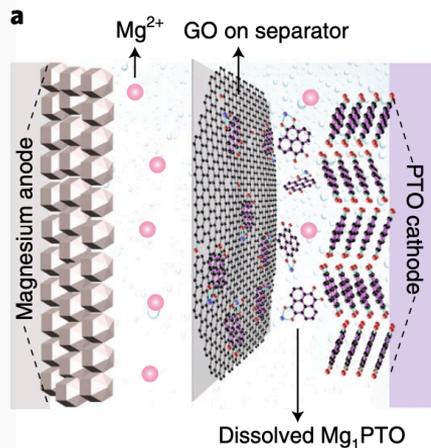
## Chemistry

enolization redox mechanism ( $C=O \leftrightarrow C-O^-$ )

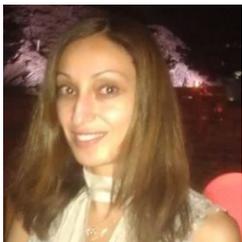


Nature Energy 5, 1043 (2020)

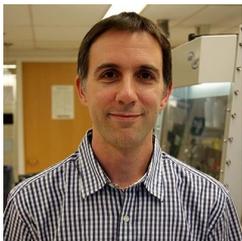
# Heterogeneous Enolization Redox Cathode Chemistry



# Electrolytes with Lower Viscosity and Weaker Coordination

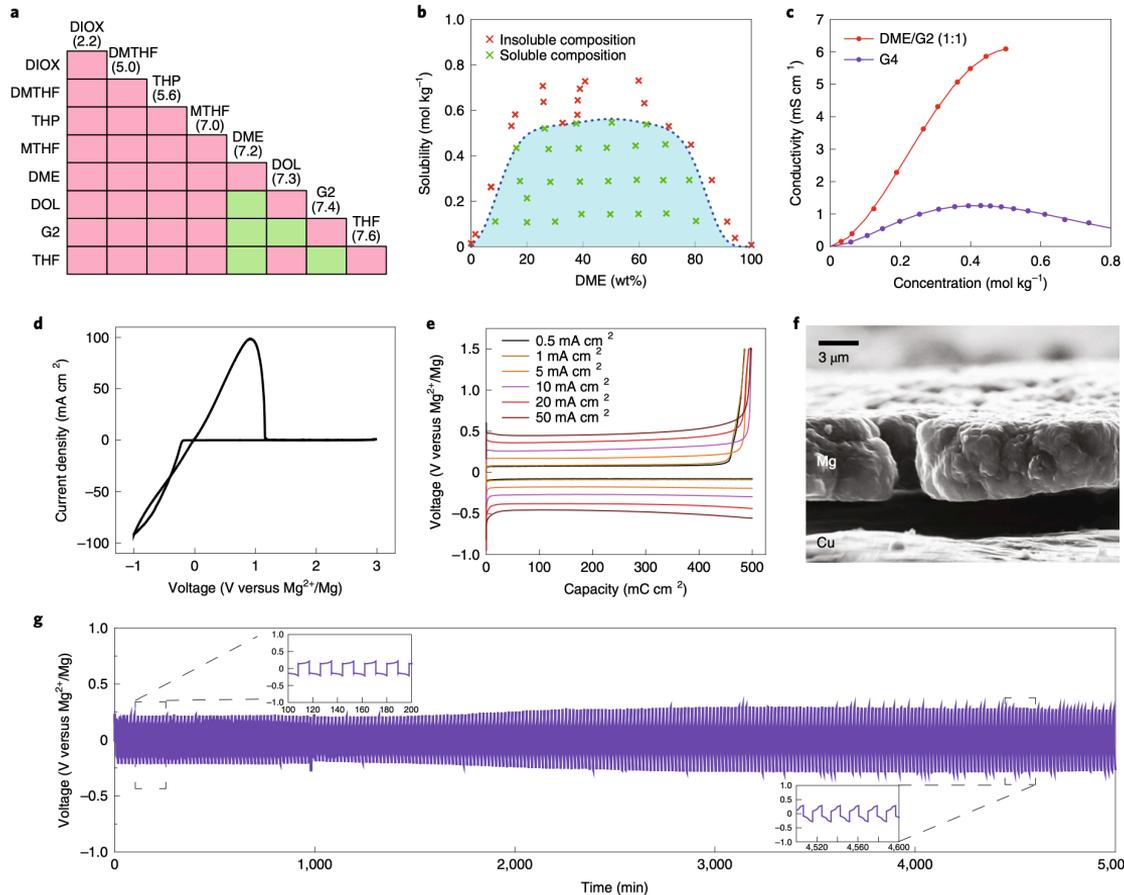


Rana Mohtadi

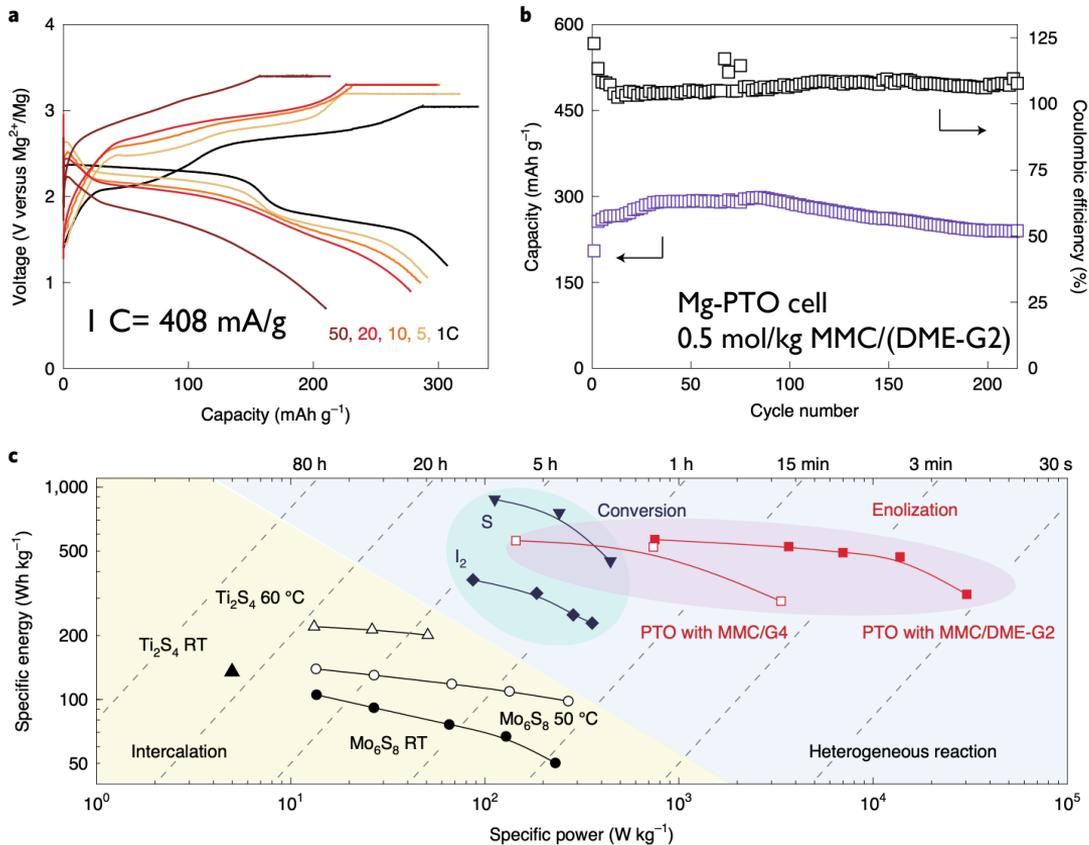


Óscar Tutusaus

TRINA



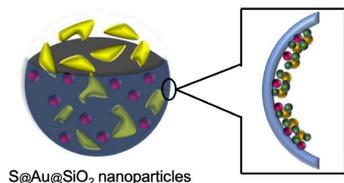
# High-power Mg Batteries



# Energy Storage Program in Yao Group

## Li-ion battery

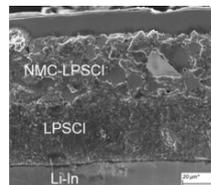
ACS AMI. ASAP (2020)  
Chem. Comm. 51,229 (2015)



S@Au@SiO<sub>2</sub> nanoparticles

## Solid-state Li battery

ACS Energy Lett. (2020)  
Joule (2020)



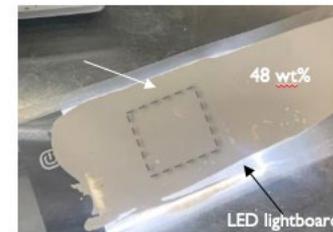
## Characterization

DOE VTO Project



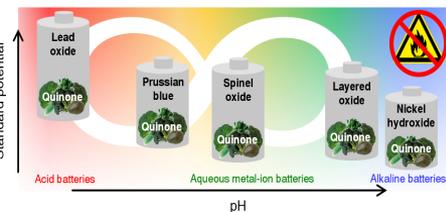
## Manufacturing

UH AMI Project



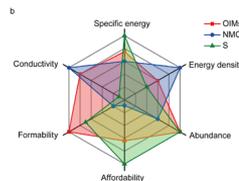
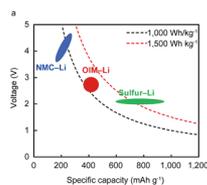
## Grid-scale storage

Nature Mater. 16, 841 (2017)



## Organic battery

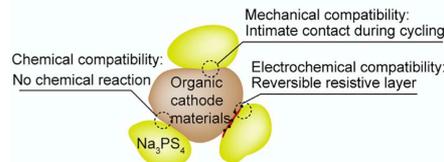
Chem Rev. 120, 6490 (2020)  
Joule 2, 1690 (2018)



## Na battery

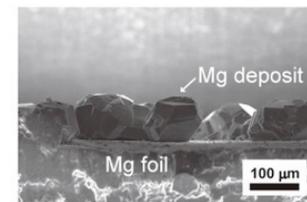
Joule 3, 1349 (2019)  
Angew Chemie 130, 2660 (2018)

Favorable electrode-electrolyte interface



## Mg battery

Nature Energy 5,1043 (2020)  
Nature Energy 5, 645 (2020)  
Nature Comm. 8, 339 (2017)



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