

Multiscale Modeling Tools: From Ab initio to Mesoscale for Dendrites in All Solid-state Batteries

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Rochester Institute of Technology, New York

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DOD-ARO-YIP

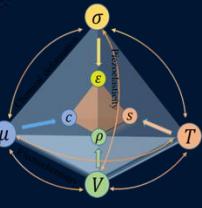


NSF-Engine



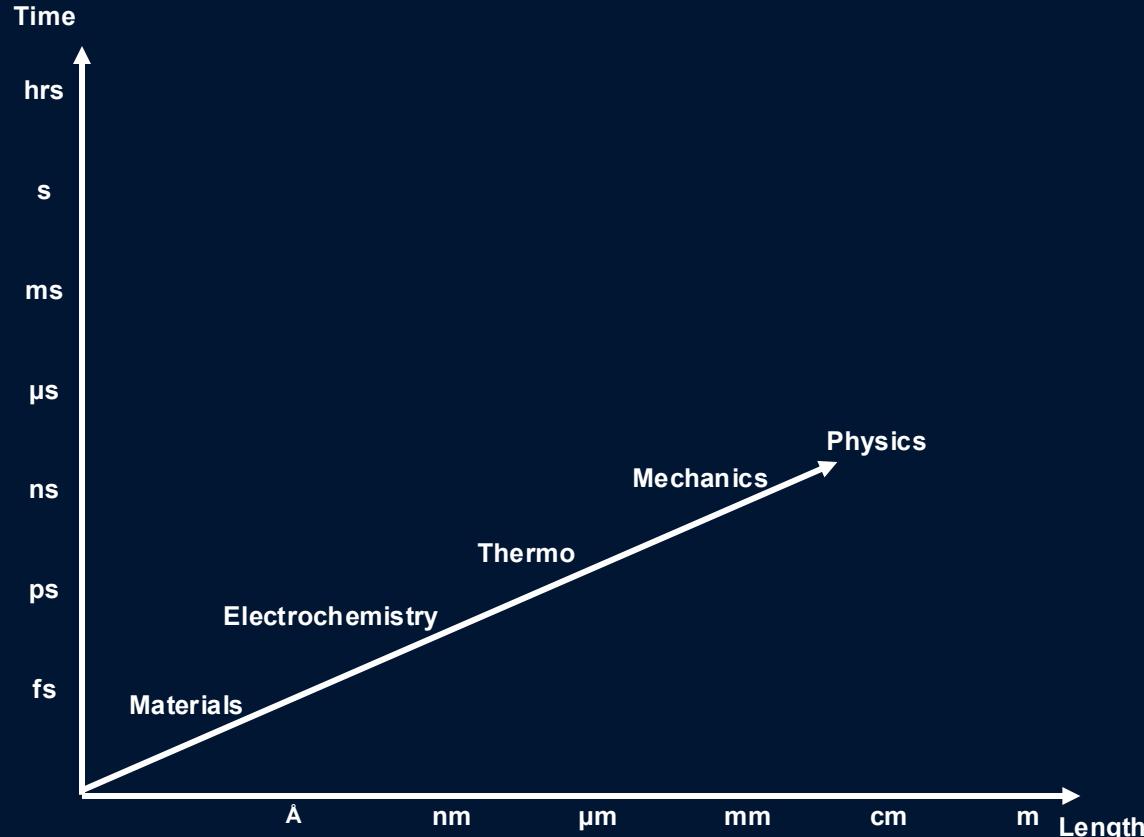
DoE-VTO (Seedling)

Thermo (T)
- Electro (V)
- Chemo (μ)
- Mechanics (σ)



Multiscale modeling for Interfaces in Solid-state Batteries

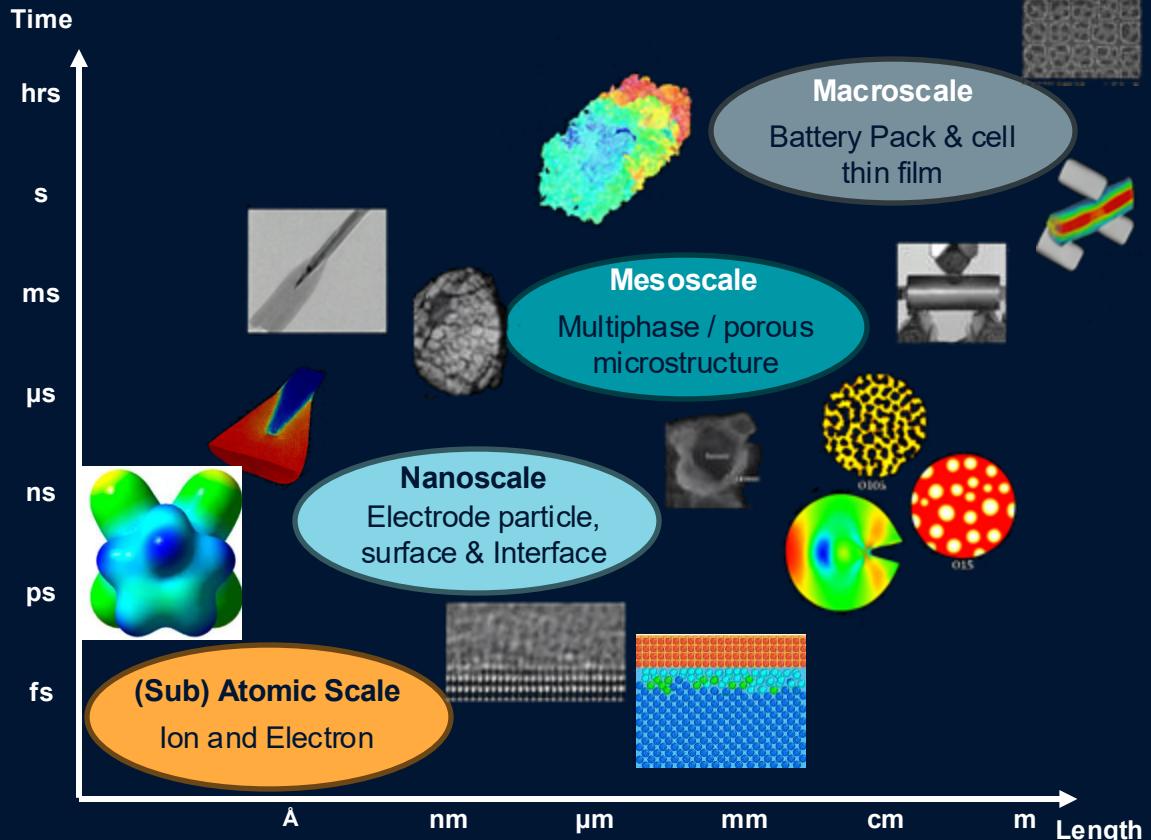
❖ Multiscale modeling



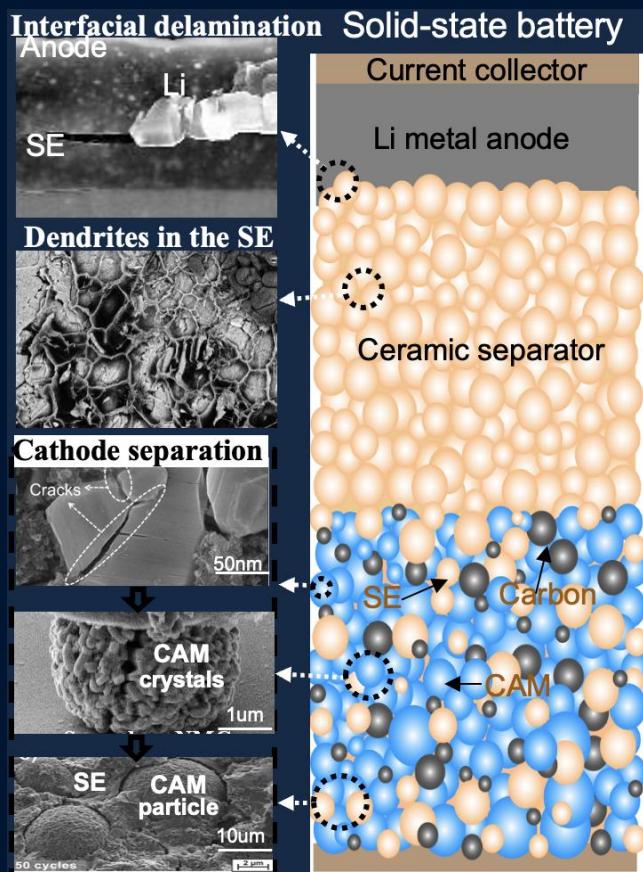
A real research project is sometimes a coupling of multi-length scale, multi-time scale, and multi=physical scale.

Multiscale modeling for Interfaces in Solid-state Batteries

❖ Multiscale modeling

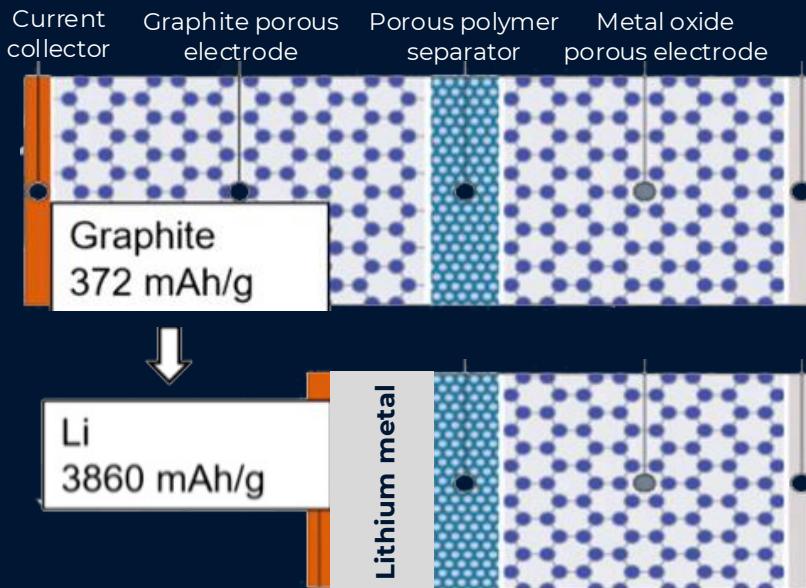


❖ Failures in Solid-state batteries

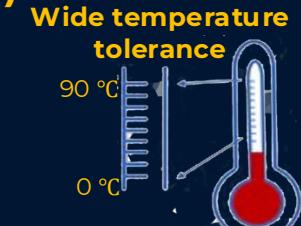
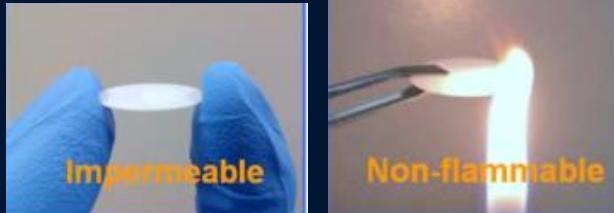


Problem Statement:
What are Dendrites in Solid-state Systems?

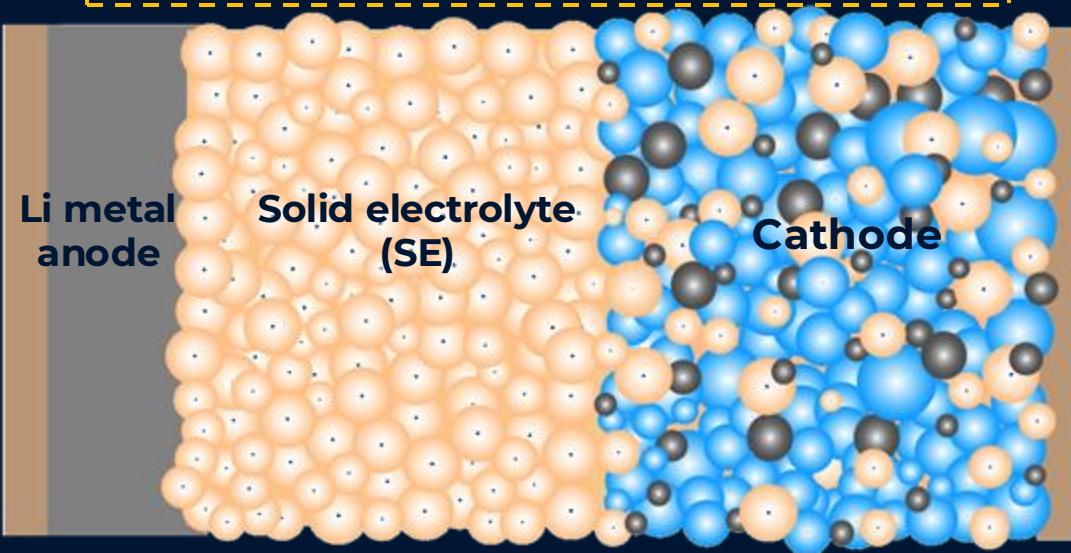
Li-ion Battery is Great but Higher Energy and Safety are Needed



❖ Inorganic solid electrolyte (ceramics)

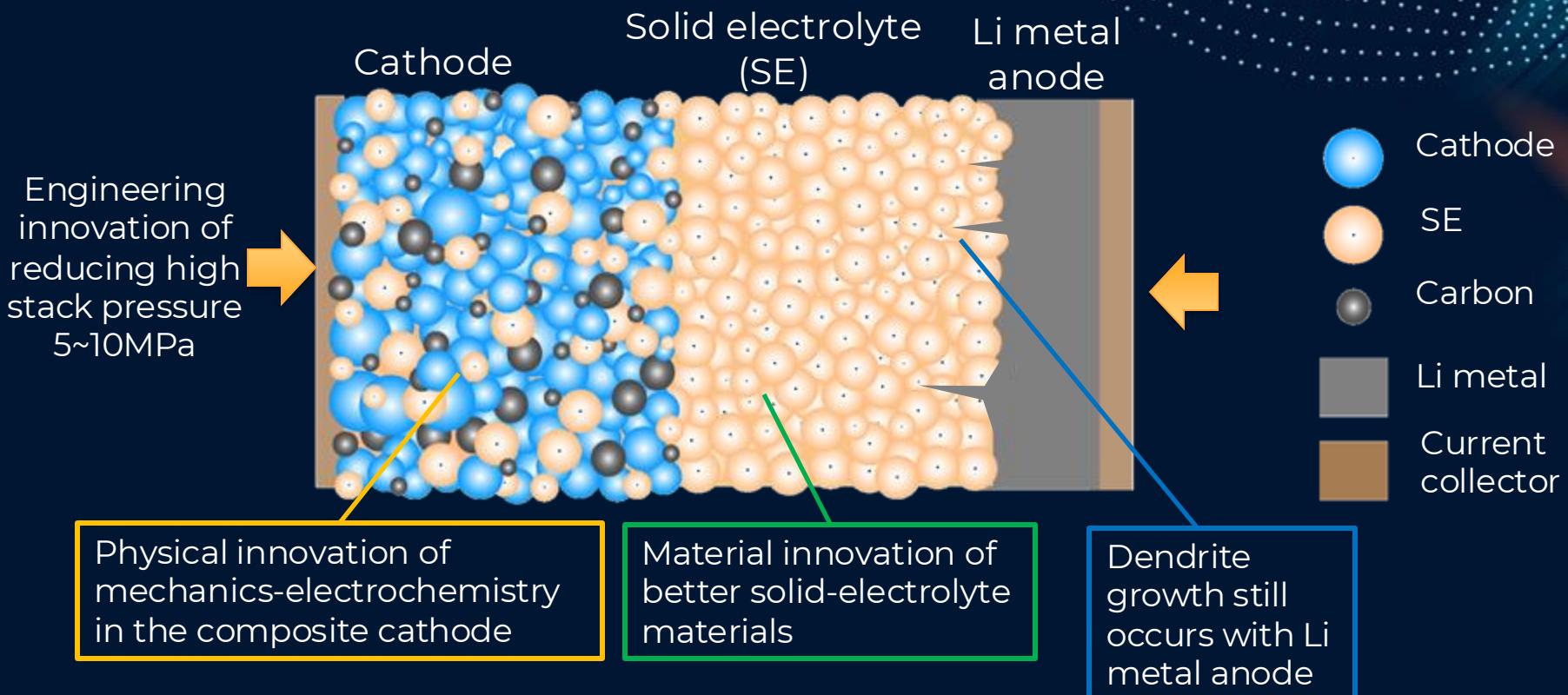


Assemble solid electrolyte and Li metal:
Solid-State Battery

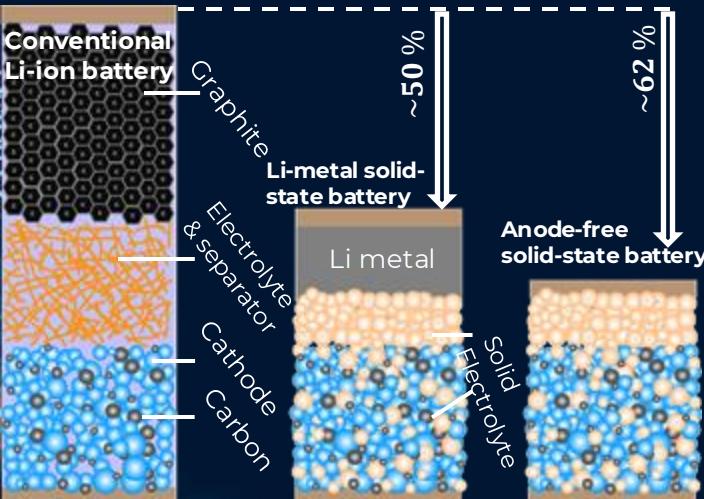


Major issue: Li metal
is unstable with most
liquid electrolytes

Challenges in solid-state batteries



My group has been working on SSB R&D many years



Dendrites issue (9)

- Luis Luque, **H. Tu**, G. Ceder et al. *ECS* 167.2 (2021).
- **H. Tu**, G. Ceder et al. *Cell Reports Physical Science* 1.7 (2021).
- **H. Tu**, G. Ceder, *Matter* 4.10, 2021.
- Peng, X., **H. Tu***, & Scott, M. C., et al. (2023) *Science Advances*, 9(17),.
- **H Tu***, S. Arkihero, et al small, 2023.
- Daxian Cao, **H Tu***, H. Zhu, et al. *Nano letter*, 2023.
- Mouhamoud, **H Tu***, G.Ceder et al. *Nature Comm* (2023).
- Yixian Wang, **H Tu***, D. Mintlin, et al. *Advanced Science*, 2024.
- Mouhamoud, **H Tu***, G.Ceder et al. *AEM* (2025). In press

Anode-free SSB (4)

- Fengyu, **H Tu***, G.Ceder et al. *AEM* (2023).
- Imtiaz S, **H Tu***, et al. *ECS* 171.9, 2024.
- Nuhu Bage, **H Tu***. *Electrochim* 5.4, 2024
- L. Zhao, **H. Tu***, Y. Yao, et al. *Nature Comm*, . In press

Solid Electrolyte (3)

- Yihan Xiao, **H. Tu**, et al. *AEM* 11.37, 2021.
- N. Szymanski, **H. Tu**, et al. *CM* 33.11, 2021.
- Zhi Dong, **H. Tu***, et al. *Nano Energy*, 2024.

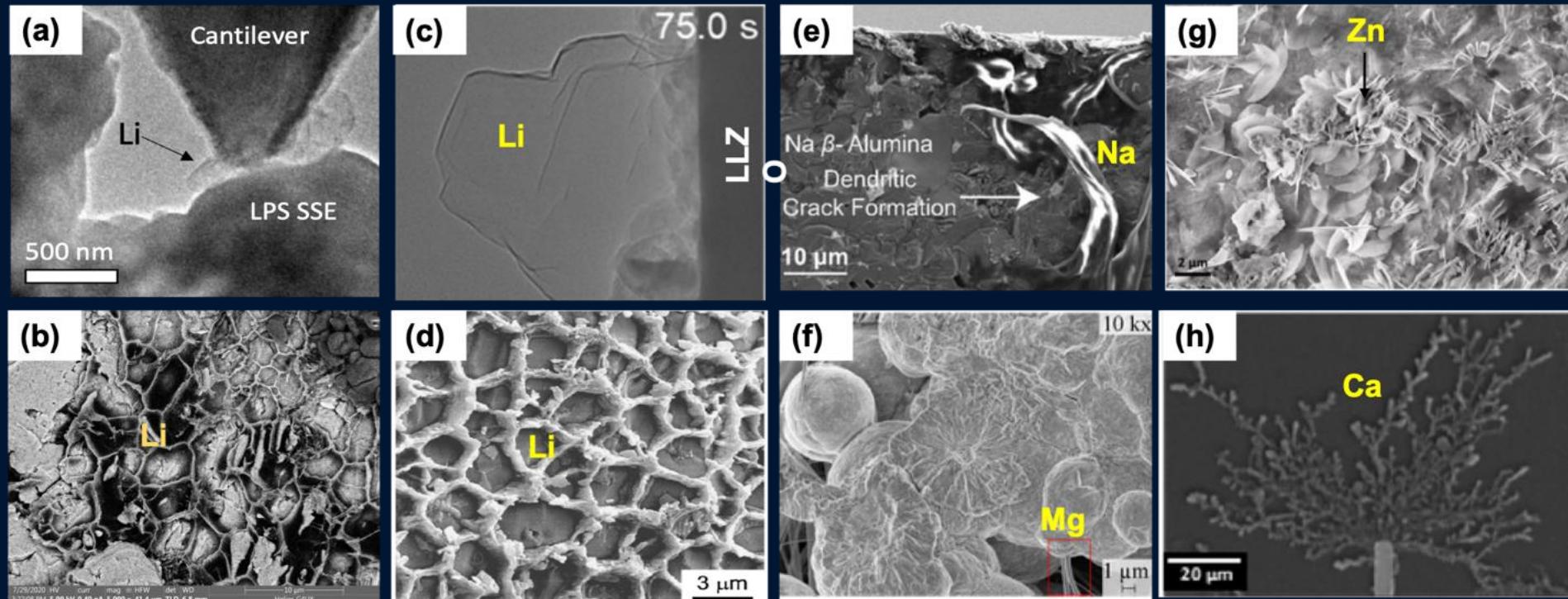
Composite Cathode (6)

- Tan Shi, **H Tu*** et al. *AEM* 10.1 (2020).
- Farzanian, Shafee, **H Tu*** et al. *ACS Applied Energy Materials* 6.18 (2023): 9615-9623.
- Tongtai Ji, **H Tu***, H. Zhu, et al. *EES*, 2024
- Nuhu Bage, **H Tu***. *J. Energy Storage*, 2024
- Yuan Y, **H Tu***, Y. Zhao et al. *Joule* (2025). In press
- Joseph V, **H Tu*** et al. *Nature Comm* (2024). In press

Patents (4)

- **H. Tu**, J.Vazquez, F. Cunez. "Method for Densification of SE." Provision filed, 2025
- H Tu, E. Velazquez. "An Open-Electrode Battery System." Provision approved, 2024
- S Chakravarthy, H Tu, et al "Solid state Cathode" US Patent App. 17/116,583, 2022
- H. Tu, et al. "SOLID POSITIVE ELECTRODE." U.S. Patent Application No. 16/459,896

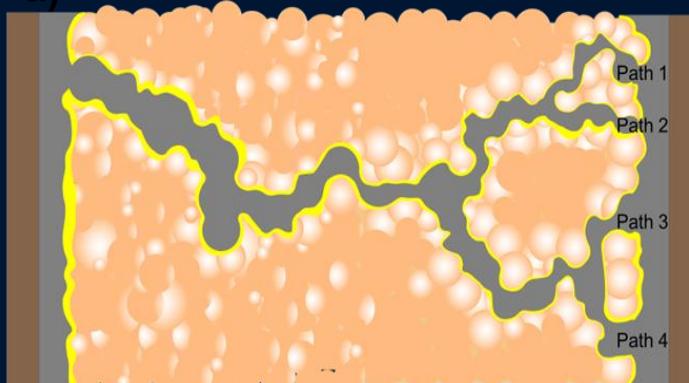
Dendrites are cancer-like issue in almost all battery systems



“Dendrites” were defined as mossy and branching structure, but are very different in solid-state systems, therefore it was also called “Li filaments”

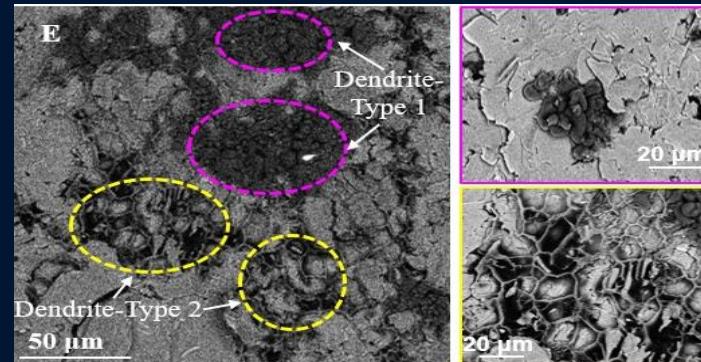
Dendrites Issue is a multiscale problem

❖ Dendrites are the inhomogeneous Li deposition during charging

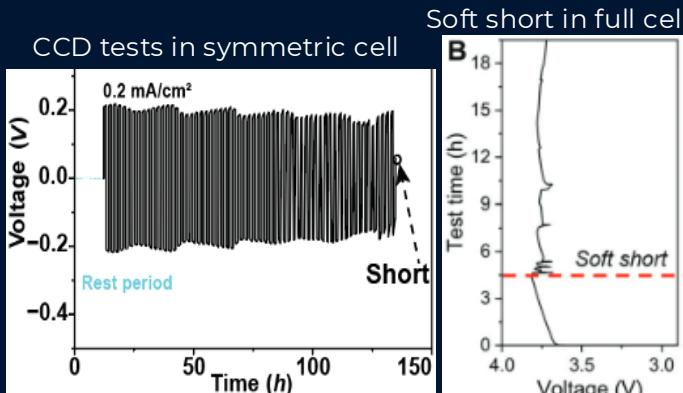


H. Tu, G. Ceder et al. *Cell Reports Physical Science* 1.7 (2020).

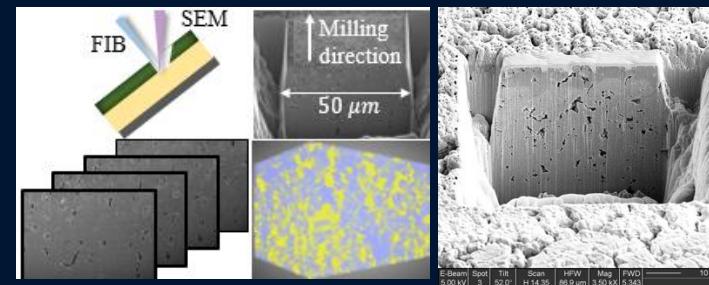
❖ Dendrites exist at multi scale, almost impossible to be suppressed but can be alleviated



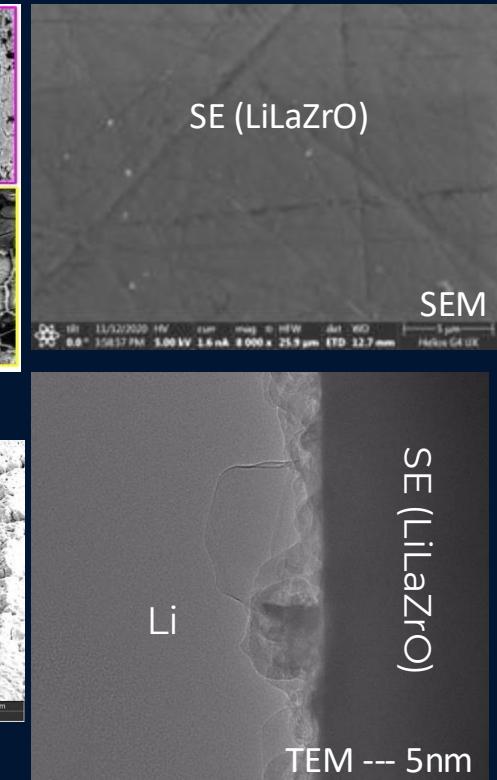
H Tu*, S. Arkihoro, et al *small*, 2023.



Mouhamoud, H Tu*, G.Ceder et al. *Nature Comm* (2023).
Adv. Funct. Mater. 2023, 33, 2307998



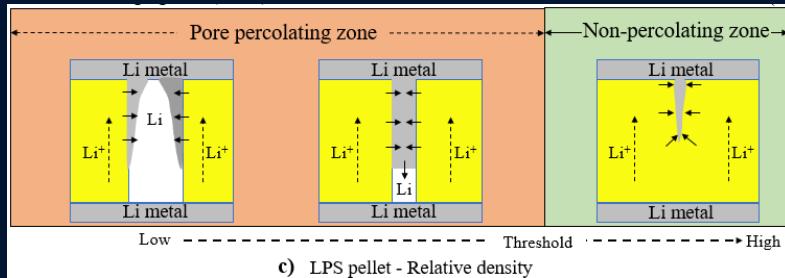
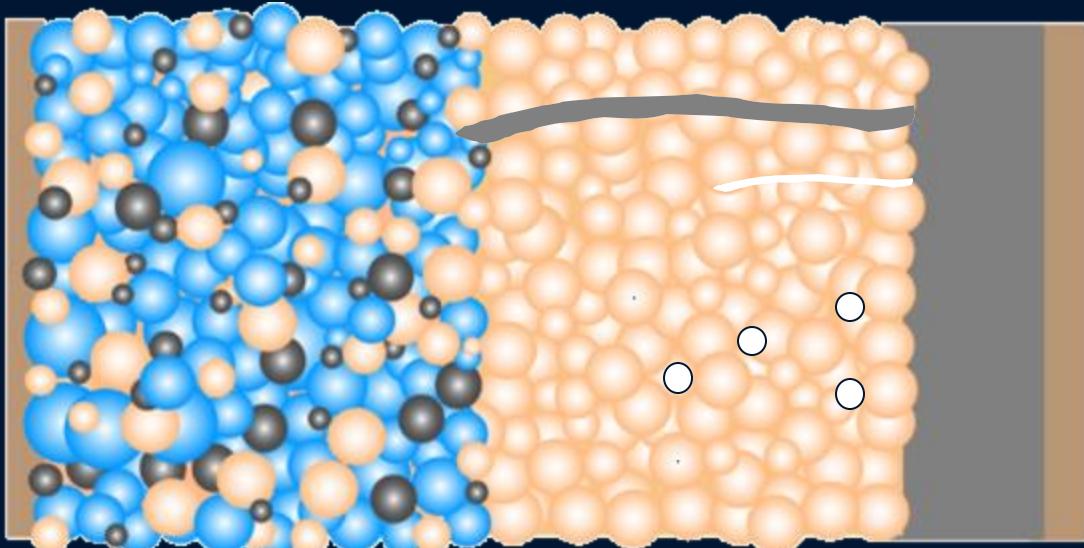
Tan Shi, H Tu* et al. *AEM* 10.1 (2020).



TEM --- 5nm

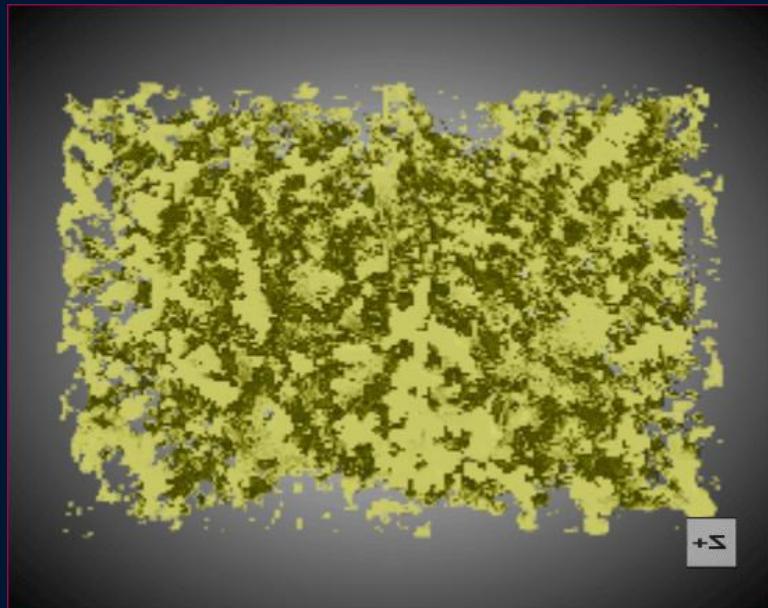
Peng, X., H. Tu*, & Scott, M. C., et al. (2023) *Science Advances*, 9(17),

Four typical mechanisms for dendrites growth

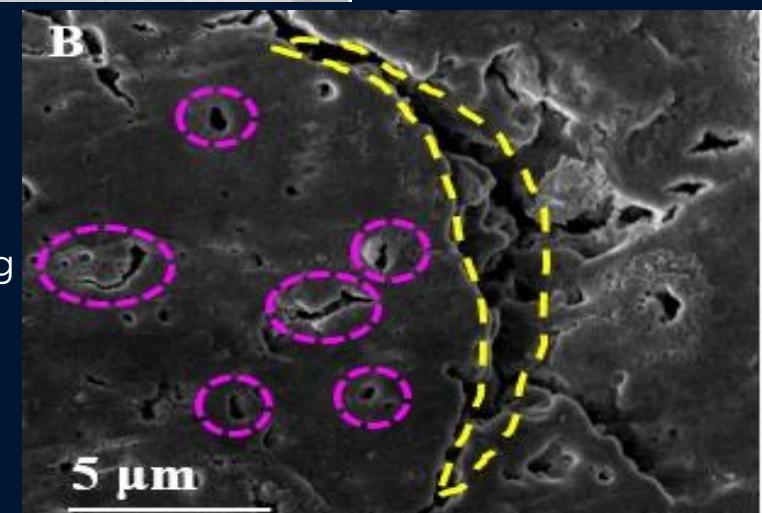
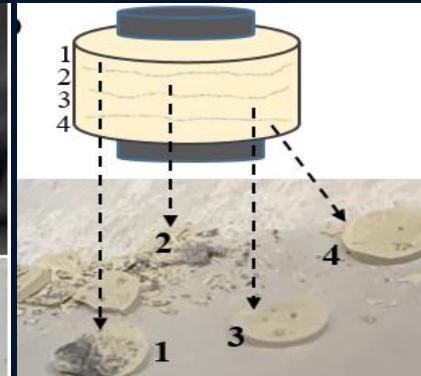
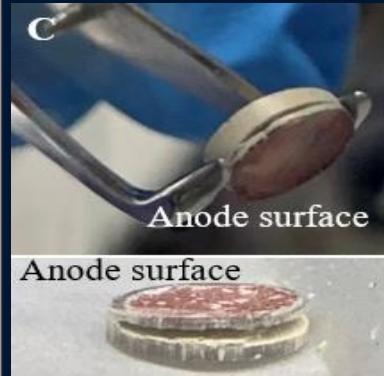
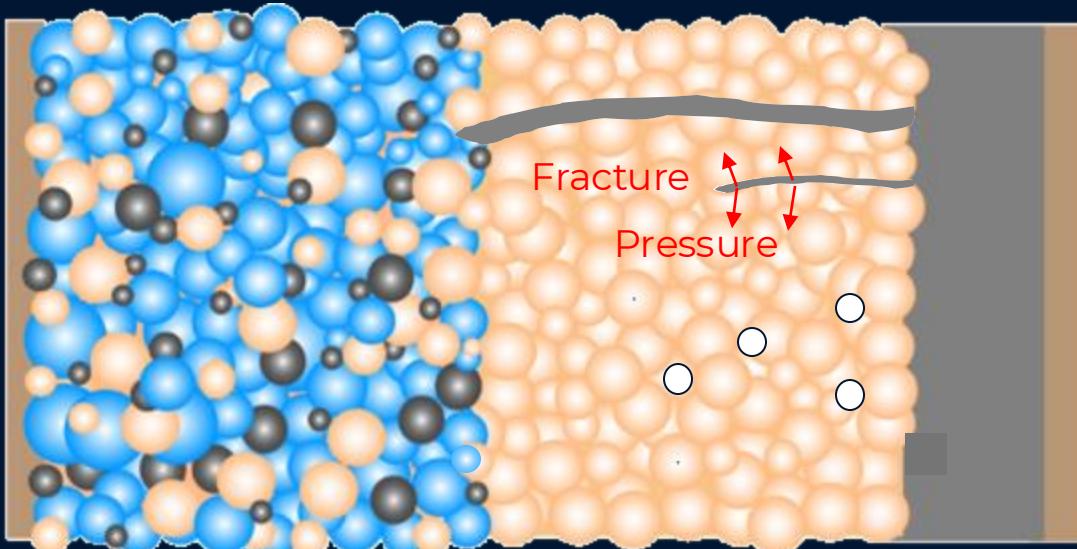


1. Percolating pores: Li simply grows through the SE

Mouhamoud, H Tu*, G.Ceder et al. *Nature Comm* (2023).



Four typical mechanisms for dendrites growth



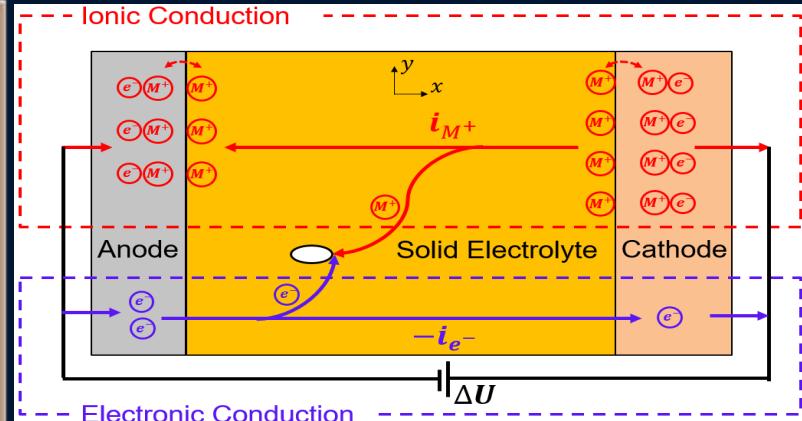
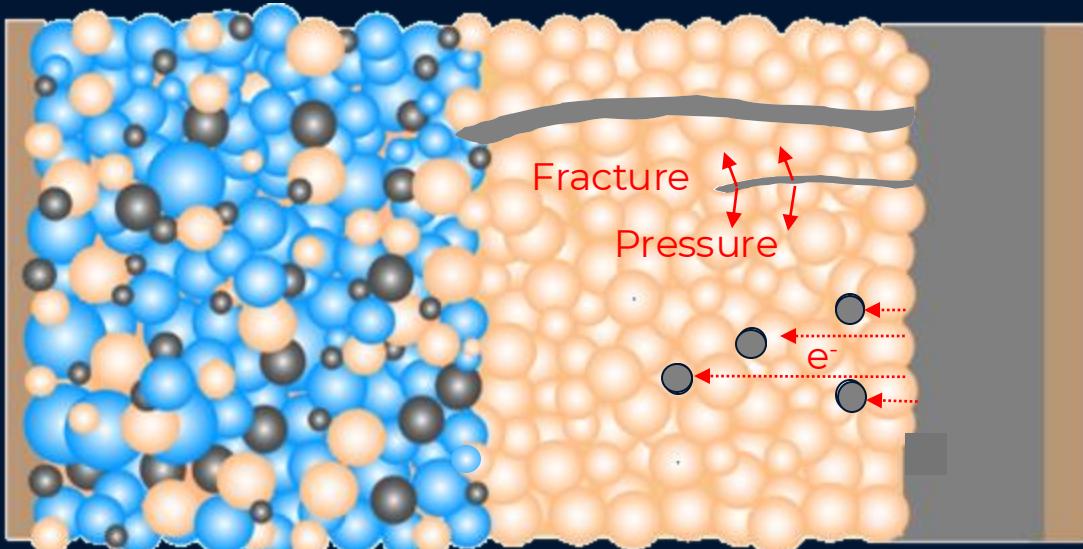
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2. Pore fracture: Stress intensification leading to propagating fracture through the grains or grain boundaries.

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Four typical mechanisms for dendrites growth



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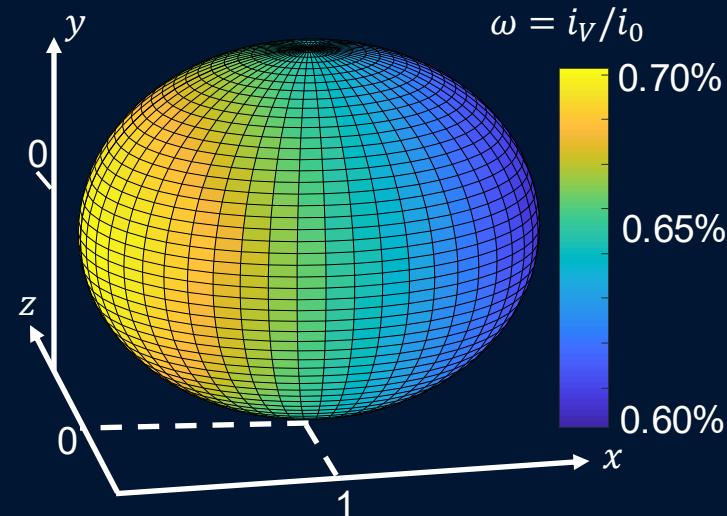
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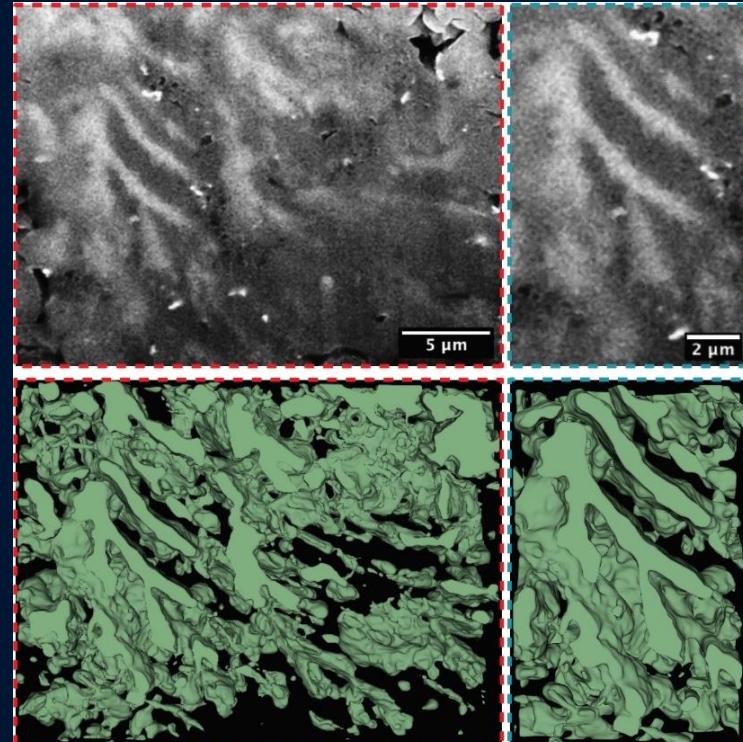
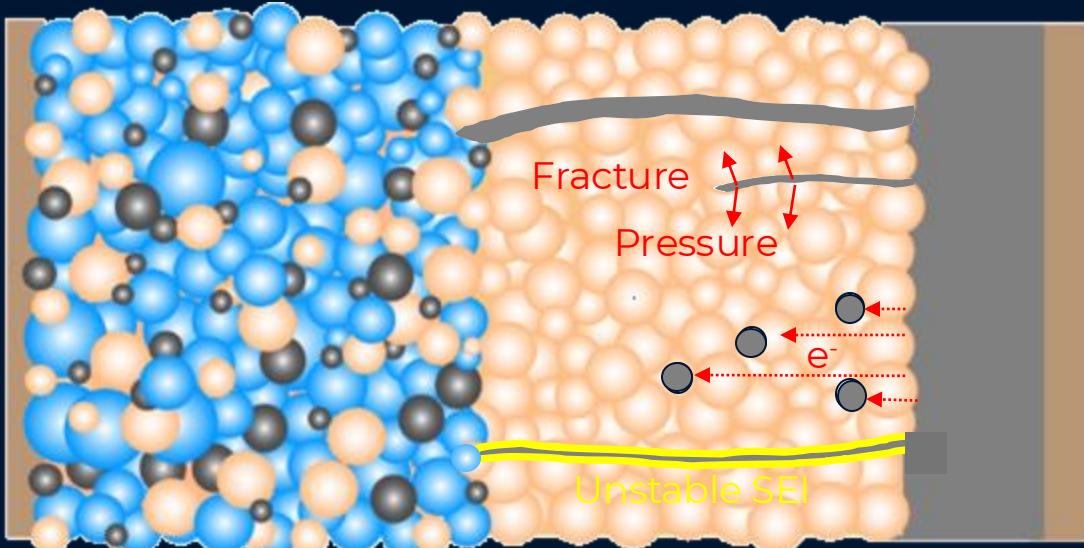
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3. Isolated porosity: Li deposits due to electronic conductivity

Qingsong Tu, et al. *Understanding Metal Propagation in Solid Electrolytes due to Mixed Ionic–Electronic Conduction*. *Matter* 2021.



Four typical mechanisms for dendrites growth



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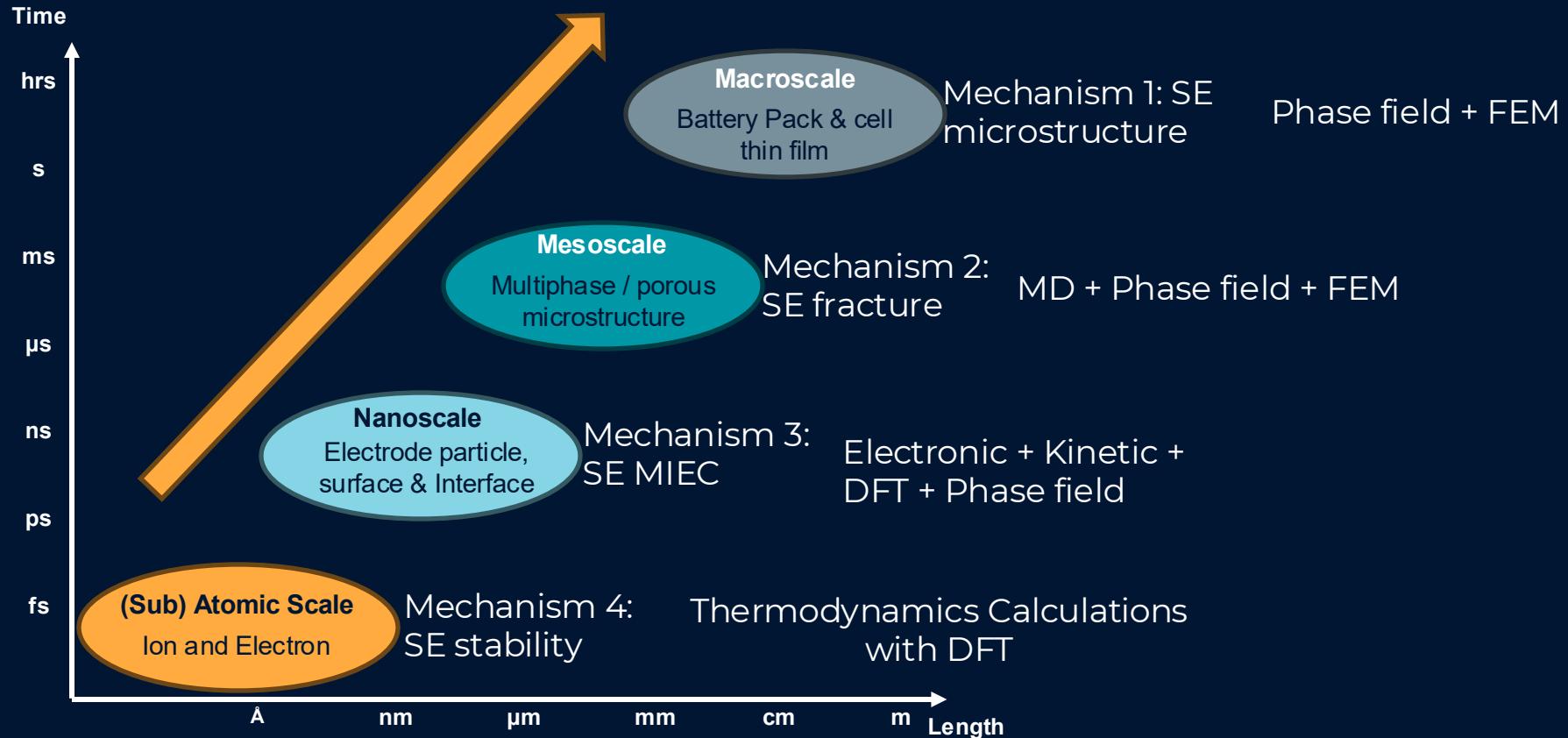
3. Isolated porosity: Li deposits due to electronic conductivity

Qingsong Tu, et al. *Understanding Metal Propagation in Solid Electrolytes due to Mixed Ionic–Electronic Conduction. Matter* 2021.

4. (Electro)chemical reactivity leading to either (1), (2) or (3).

Mouhamoud, H Tu*, G.Ceder et al. *AEM* (2025). In press

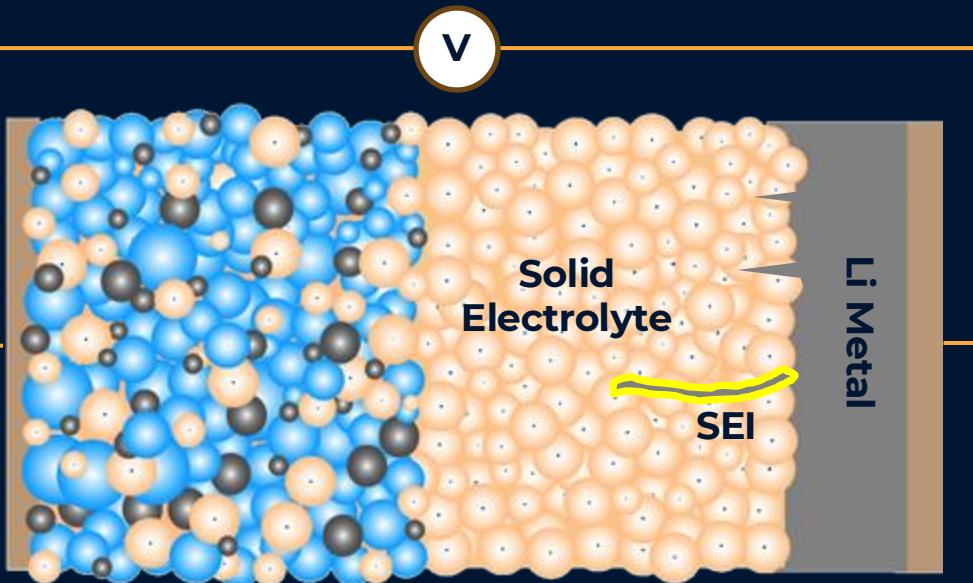
Multiscale modeling for dendrite formation & growth



**Mechanism 4: Dendrite formation due to
unstable SEI layers between Li metal and SE**

DFT calculation of the electrochemical stability of SE materials

- The solid electrolyte gets reduced at the anode side, due to high Li chemical potential of Li metal

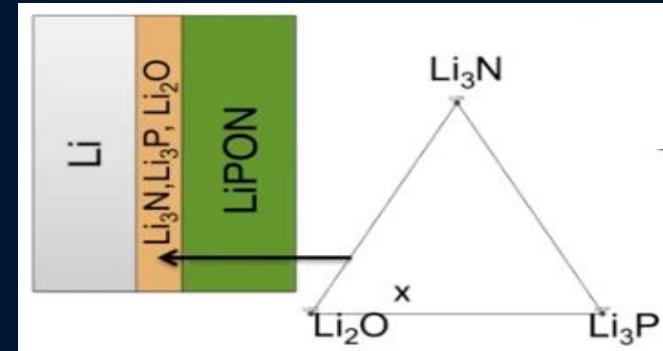


Dr. Yifei Mo's group:

10.1002/aenm.201501590

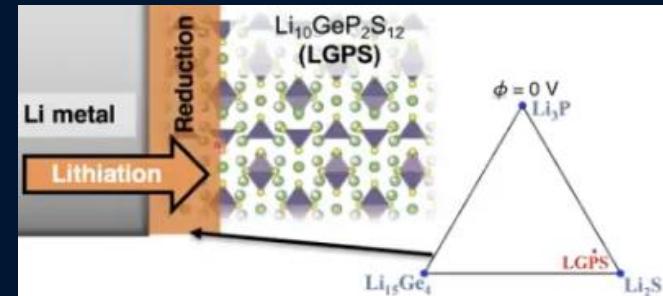
10.1021/acsami.5b07517

- Example of stable SEI



Formatted SEI layer (Li₃P, Li₃N, Li₂O) is **passivate**: ionic conducting but electronic insulating.

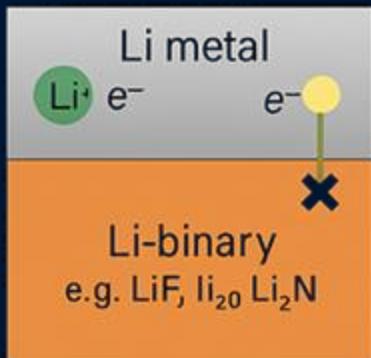
- Example of unstable SEI



Formatted SEI layer (Li₃P, Li₂S at zero voltage) is **conductive**: electronic conducting.

Material design principle for SE to prevent dendrites in SSB

Type 1 interface:
compatible
Stable, no decomposition



e.g.
 $\text{Li-G}'$ Li_2O , Li-LiLiATO

Good but rare

Type 2 interface:
non-compatible
form mixed ionic electronic (MIEC) interphase layer



e.g.
 Li_0LGPS , LiLLTO

Avoid!
Decomposition
continue!

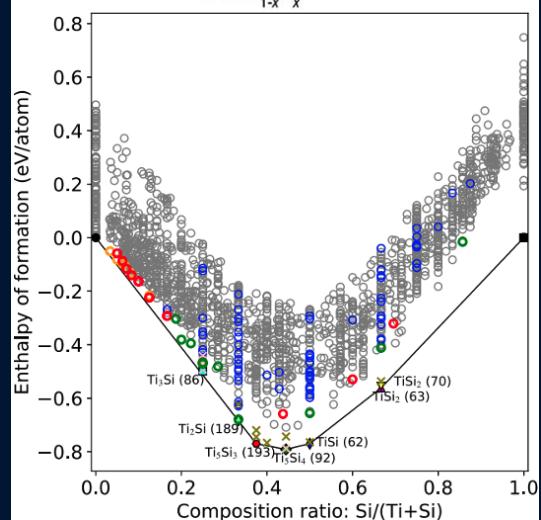
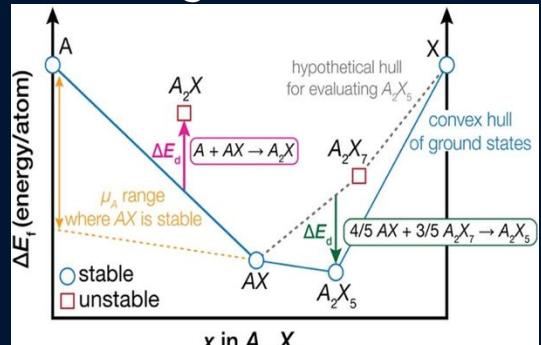
Type 3 interface:
compatible
by forming passivatin SEI layer



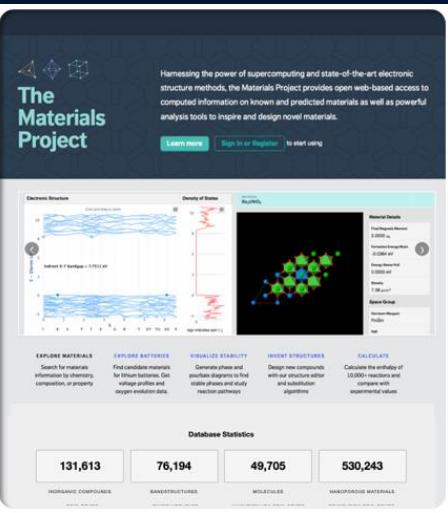
e.g.
Desired SEI property:
Ion conducting but
electronic insulating

DFT Calculation of the grand potential phase diagram with tools

❖ Phase diagram from convex hull



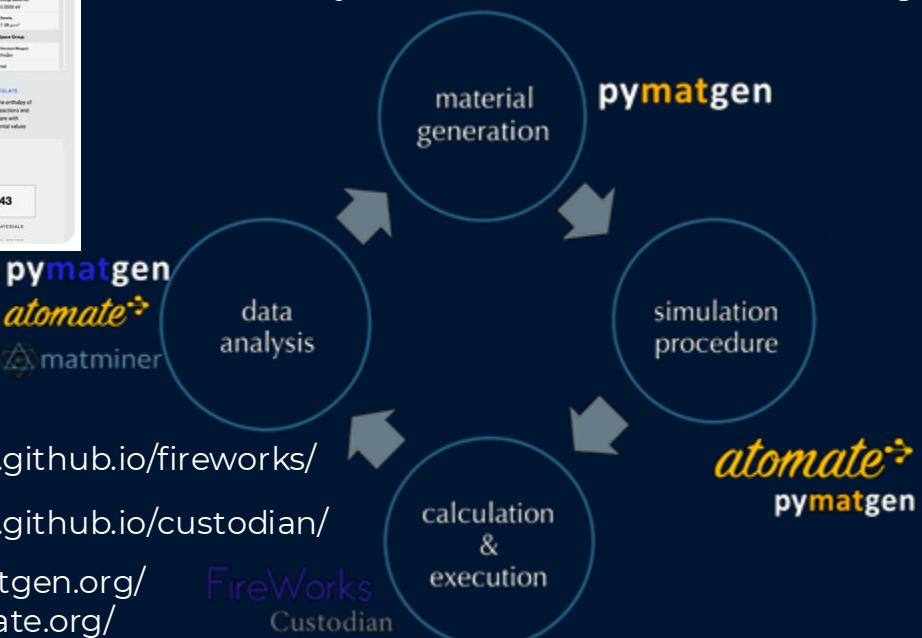
❖ Material Project contains millions of phase diagram



<https://next-gen.materialsproject.org/>

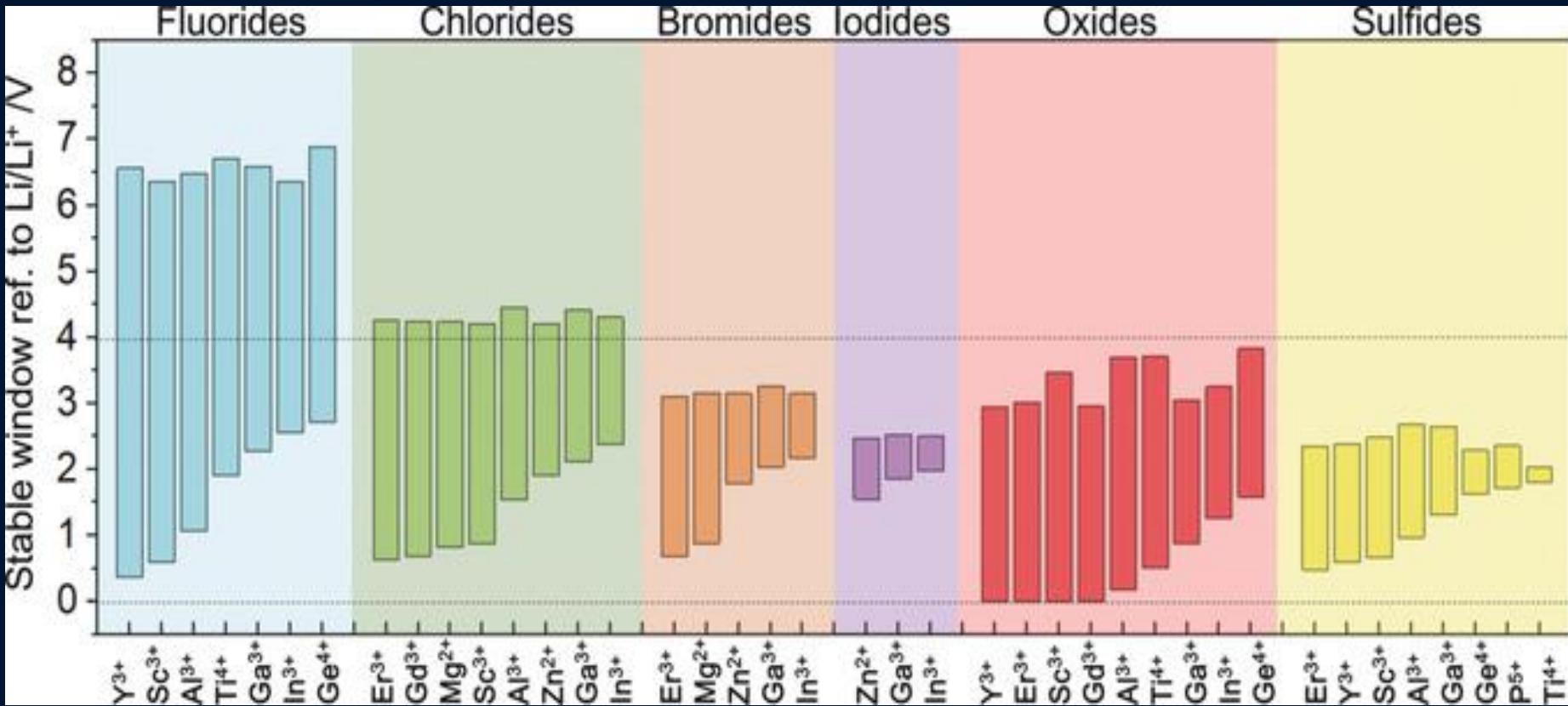
❖ Autonomous DFT calculations with open-source tools

<https://www.youtube.com/watch?v=b0tieiedGdg>



SE materials show different stability against Li formation

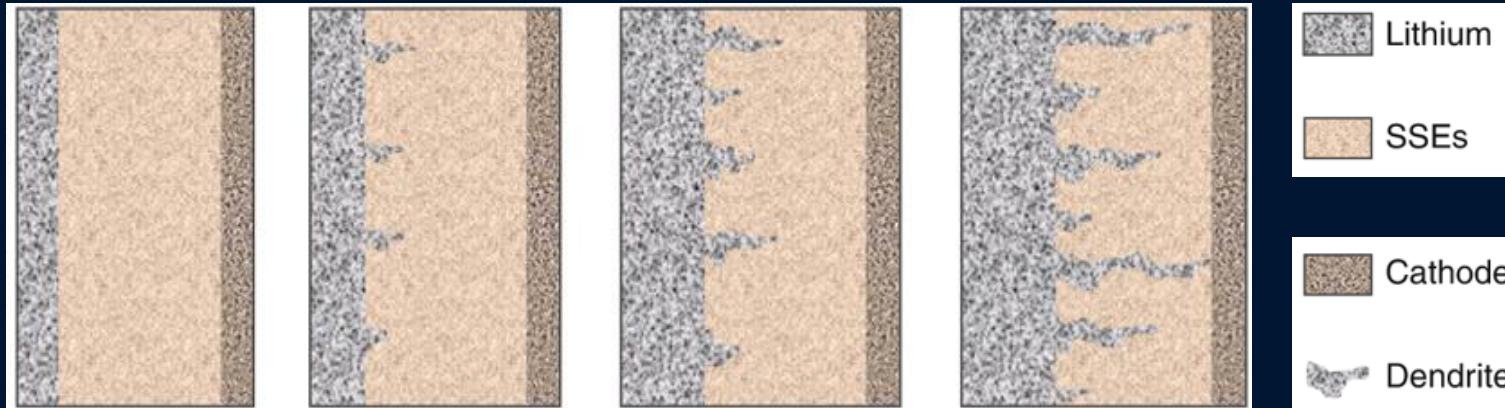
❖ Ternary compound Li-M-X (M=cation, X=F, Cl, Br, I, O, S, N)



**Mechanism 3: Dendrite formation due to
electronic conductivity of the SE**

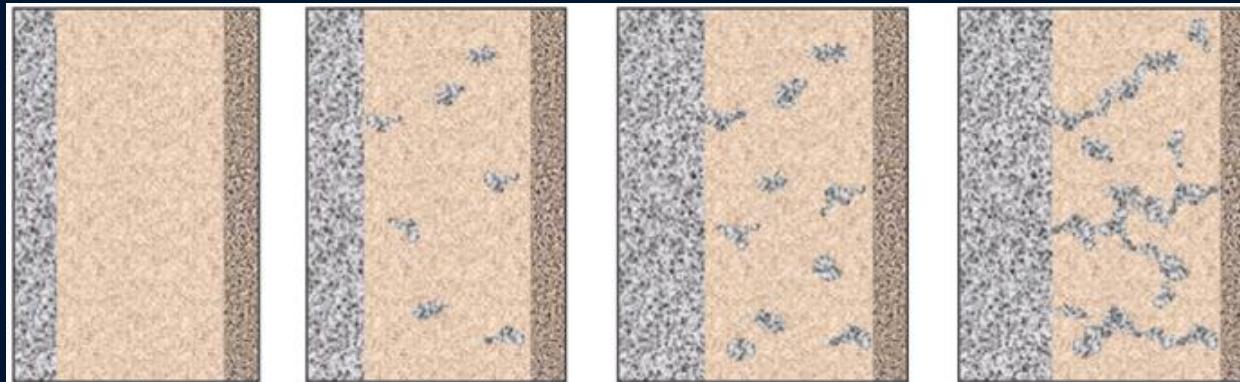
Electronic conductivity-induced mechanism

❖ Conventional interface-controlled mechanism



❖ Electronic conductivity-induced mechanism

Yu-Guo Guo, etc. The devil is in the electron. *Nature Energy*. 2019.

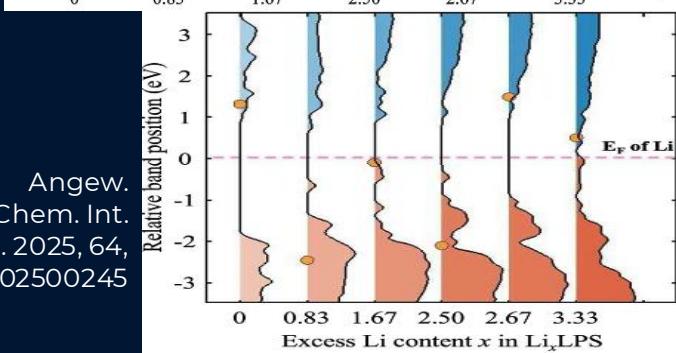
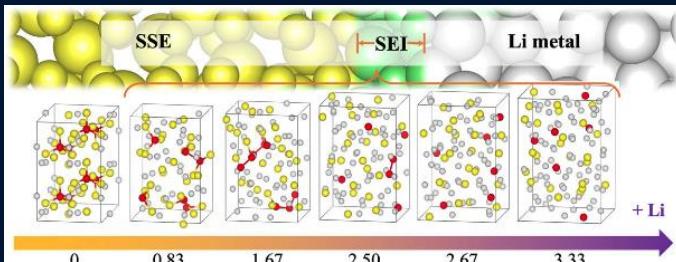
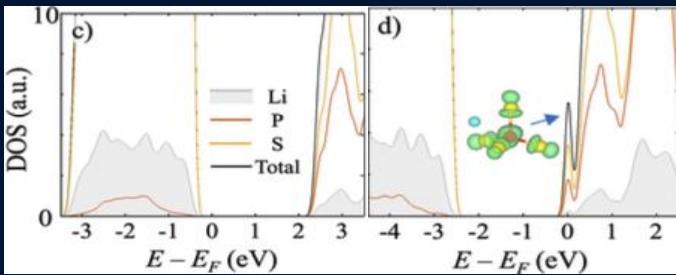


❖ Break-down Questions:

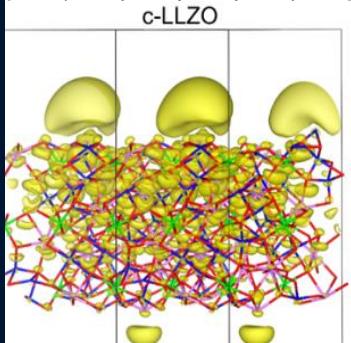
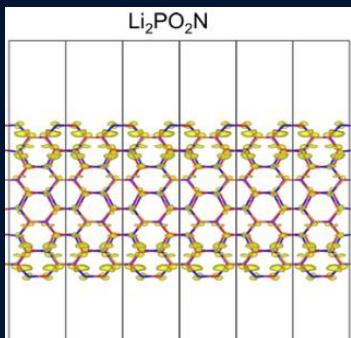
1. What is the origin of SE electronic conductivity?
2. Is the electronic conductivity ($\sim 10^{-6} \text{ mS/cm}$) enough to cause dendrite growth?

Electronic conductivity origins from electronic structure of SE

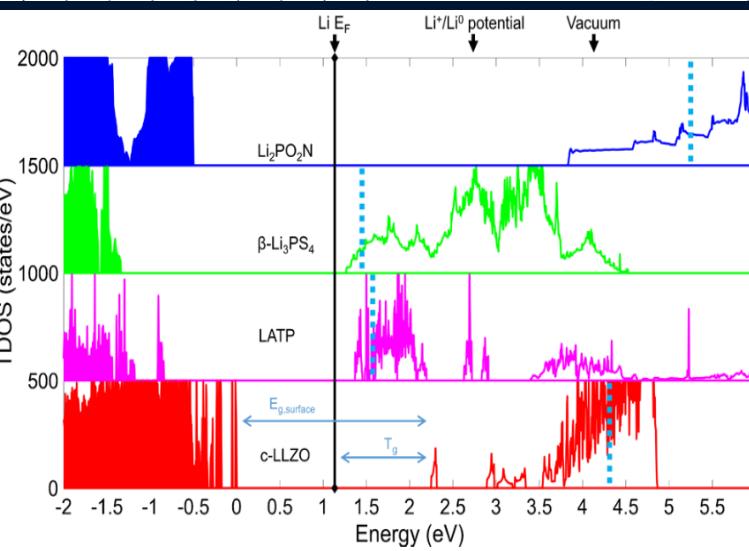
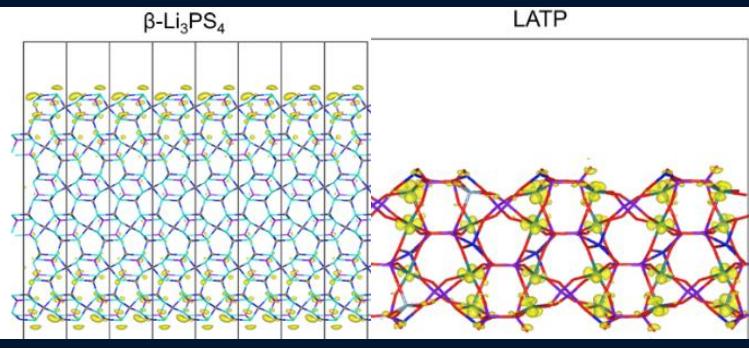
- ❖ Band gap calculation of bulk Li_xLPS
- ❖ Band gap calculation of bulk Li_xLPS



Angew.
Chem. Int.
Ed. 2025, 64,
e202500245



Chem. Mater. 2019,
31, 7351–7359



Electronic conductivity is evaluated through defect calculation

❖ Electronic conductivity calculation

$$\sigma = n_0 q \mu_n + p_0 q \mu_p$$

where n_0 and p_0 are the concentrations of free electrons and holes respectively, q is the magnitude of charge of each carrier species, and μ_n and μ_p are the electron and hole mobilities.

$$n_0 = \int_{E_{CBM}}^{\infty} \frac{1}{e^{(E-E_F)/k_B T} + 1} g(E) dE,$$
$$p_0 = \int_{-\infty}^{E_{VBM}} \left(1 - \frac{1}{e^{(E-E_F)/k_B T} + 1}\right) g(E) dE$$

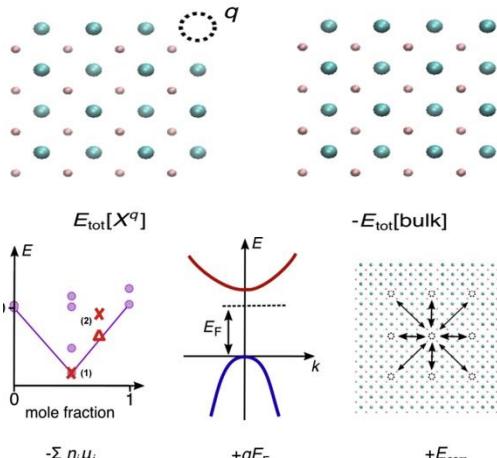
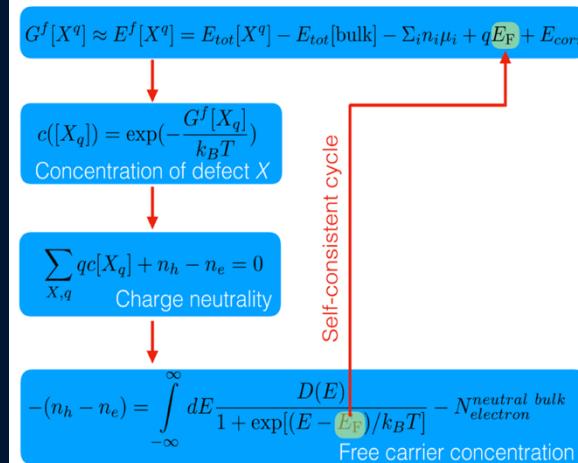
• Point defect concentrations:

$$[X^q] = N_0^X \exp\left(-\frac{\Delta E_f^{X,q}[E_F, \Delta \mu_i]}{k_B T}\right),$$

where N_0^X is the density of available sites for defect X , $E_f^{X,q}$ is the formation energy of defect X in charge state q , and μ_i are the chemical potentials of any atomic species.

$$\rho(E_F) = \sum_{X^q} q[X^q] + p_0 - n_0 = 0.$$

❖ PyCDT automatic defect calculations

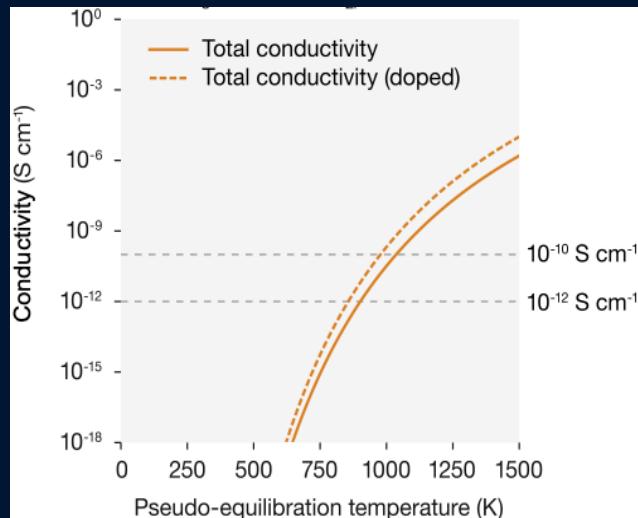


Python Charge Defects Toolkit (PyCDT) is a python package aimed at making charged defects modeling simpler, high throughput ready, and also accessible to researchers who don't have the required background. PyCDT can handle thermodynamic calculations and error corrections in the context of periodic boundary condition density functional calculations of charged defects in semiconductors and insulators.

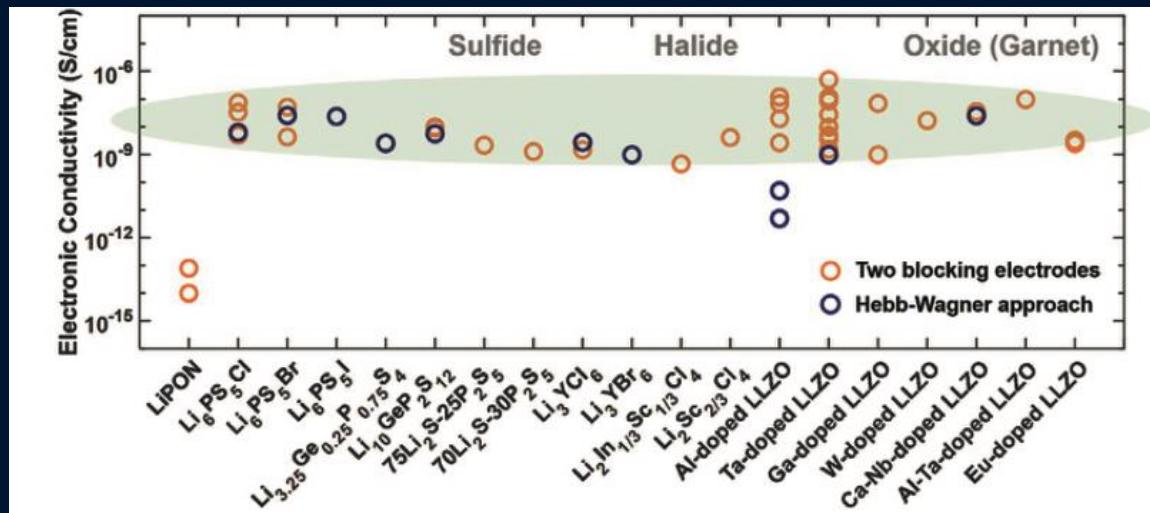
<https://github.com/mbkumar/pycdt>

Most SE materials show limited electronic conductivities

- DFT calculated electronic conductivity of LLZO



- Experimentally measured electronic conductivity of typical SE materials

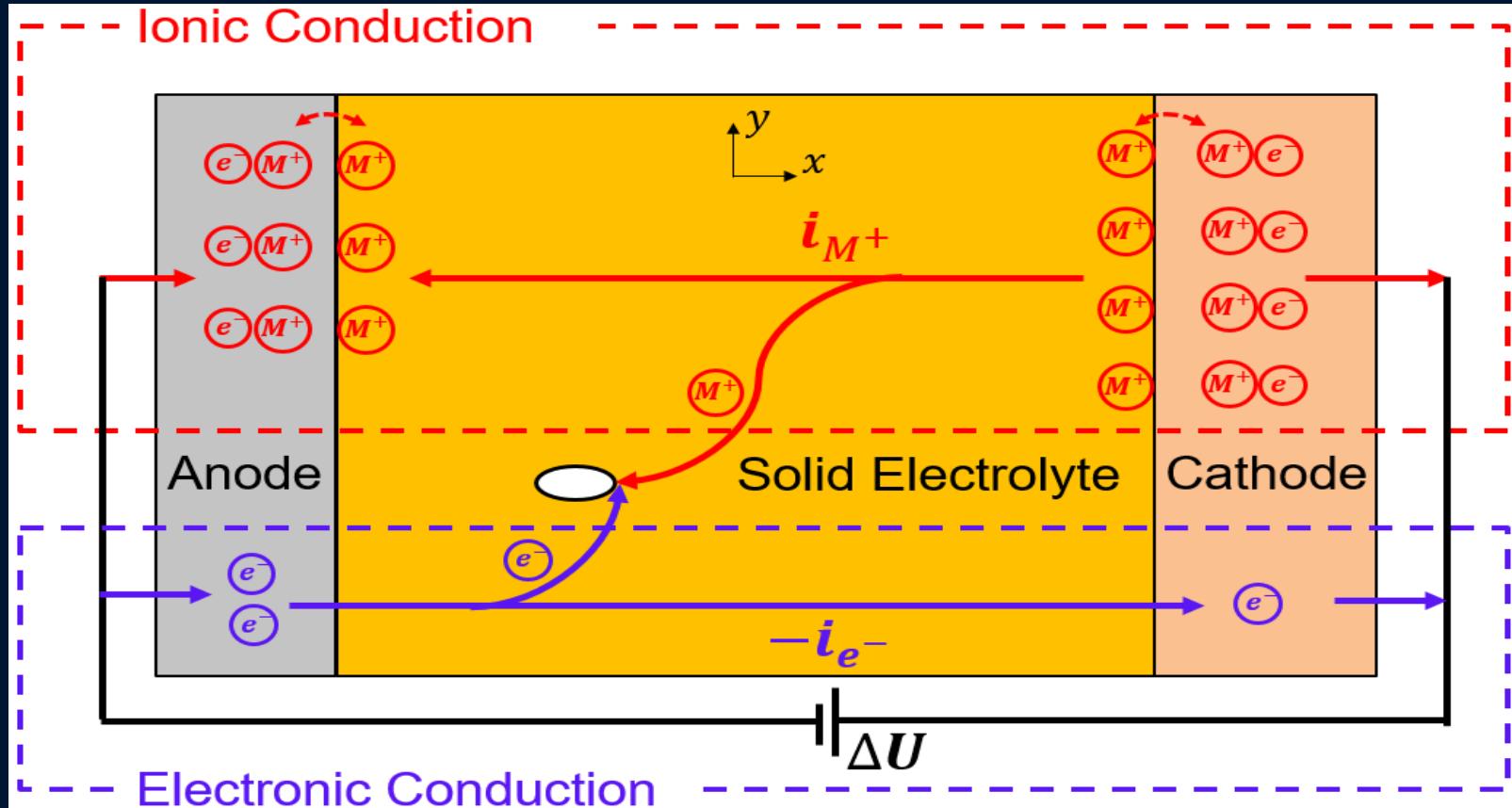


Physical Review Materials 6.8 (2022): 085401.

Adv. Energy Mater. 2023, 13, 2204098

Electronic conductivities are 4~6 order of magnitude smaller than their ionic conductivities. Will such a small value really play a role in Li dendrite formation?

Dendrite formation due to electronic conductivity of electrolyte



Methodology of the Mixed Ionic-Electronic Conductor model

1. Charge-transfer kinetics at the Anode/SE and Cathode/SE interface can be described by Butler-Volmer relation:

$$i_n^k = i_{exc}^k \left(e^{\frac{\alpha_a F \eta_k}{RT}} - e^{-\frac{\alpha_c F \eta_k}{RT}} \right)$$

- i_n^k is the surface current across the electrode/SE interfaces (k = “anode” or “cathode”).
- η_k is the surface overpotential: the drop of electrochemical potential of Li^+ ($\tilde{\mu}_{M^+}$) at the electrode/SE interface.
- η_k is defined as negative for cathodic reaction (plating: $M^+ + e^- \rightarrow M$).

2. Transport of Li^+ and e^- in the SE can be described by Ohmic relation:

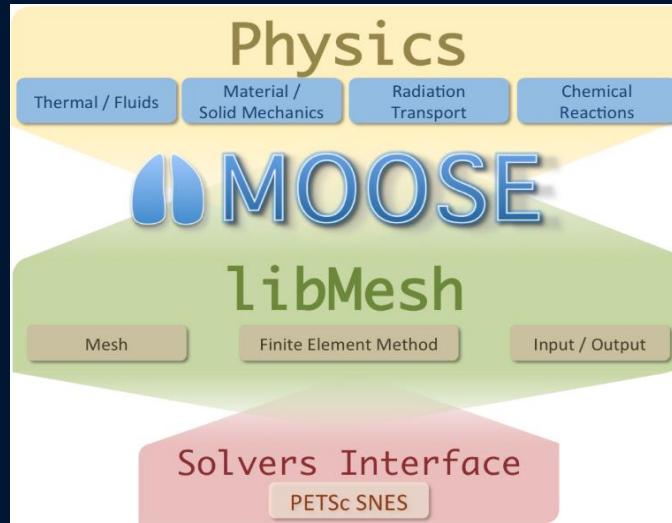
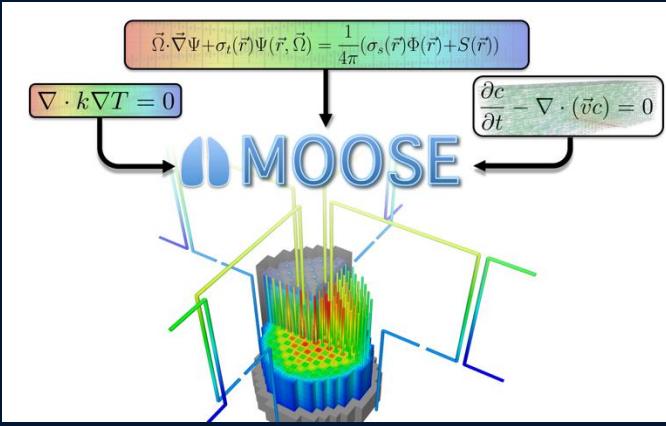
- Relation of current density (i_{M^+}, i_{e^-}) and electrochemical potential ($\tilde{\mu}_{M^+}, \tilde{\mu}_{e^-}$):

$$i_{M^+} = -\frac{\sigma_{M^+}}{F} \nabla \tilde{\mu}_{M^+}, \quad i_{e^-} = \frac{\sigma_{e^-}}{F} \nabla \tilde{\mu}_{e^-}$$

- Laplacian equation of electrochemical potential ($\tilde{\mu}_{M^+}, \tilde{\mu}_{e^-}$) at steady state:

$$\nabla^2 \tilde{\mu}_{M^+} = 0, \quad \nabla^2 \tilde{\mu}_{e^-} = 0$$

MOOSE framework can be used to solve transport equations



Strong Form

$$\rho C p \frac{\partial T}{\partial t} - \nabla \cdot k(T, B) \nabla T = f$$

Weak Form

$$\int_{\Omega} \rho C p \frac{\partial T}{\partial t} \psi_i + \int_{\Omega} k \nabla T \cdot \nabla \psi_i - \int_{\partial \Omega} k \nabla T \cdot \mathbf{n} \psi_i - \int_{\Omega} f \psi_i = 0$$

Kernel Kernel BoundaryCondition Kernel

Actual Code

```
return _k[_qp]*_grad_u[_qp]*_grad_test[_i][_qp];
```

MOOSE Modules

Physics

Chemical Reactions

Contact

Electromagnetics

Fluid Structure Interaction (FSI)

Geochemistry

Heat Transfer

Level Set

Navier Stokes

Peridynamics

Phase Field

Porous Flow

Solid Mechanics

Thermal Hydraulics

Numerics

External PETSc Solver

Function Expansion Tools

Optimization

Ray Tracing

rDG

Stochastic Tools

XFEM

Physics support

Fluid Properties

Solid Properties

Reactor

<https://doi.org/10.1016/j.softx.2025.102264>

<https://github.com/idaholab/moose>

<https://mooseframework.inl.gov/index.html>

1D analytic solutions shows the Li deposition current in the void

❖ Charging of symmetric cell

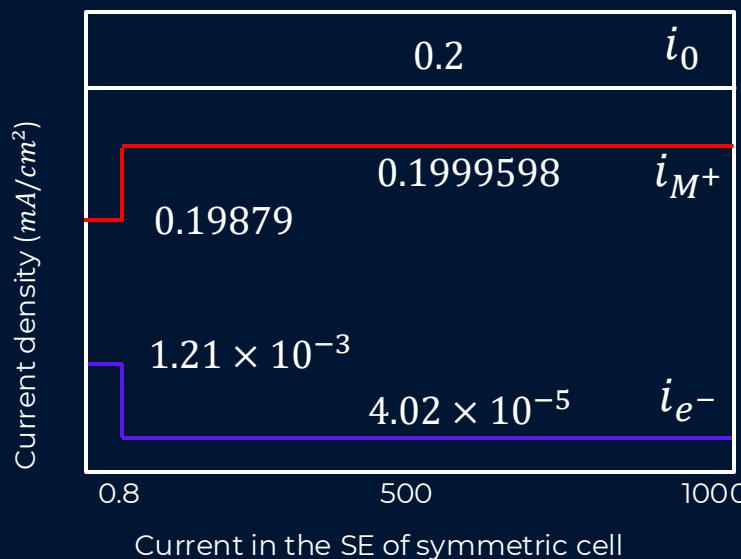


❖ Analytic solution for deposition current in the void

$$i_V = \frac{\left(\frac{R_C}{R_e} + \frac{L-a}{L}\right) \frac{\mu_M^A}{FR_A} + \left(\frac{R_A}{R_e} + \frac{a}{L}\right) \frac{\mu_M^C}{FR_A} + \left(\frac{L-a}{L} - \frac{R_C a}{R_A L}\right) i_0}{\frac{R_C}{R_e} + \frac{L-a}{L} + \frac{R_V}{R_e} + \frac{R_V}{R_A} + \frac{R_V R_C}{R_e R_A} + \frac{R_C a}{R_A L} + \frac{R_e a(L-a)}{R_A L^2}}$$

Expression	Description	Value
$i_t (\text{mA/cm}^2)$	External C.D.	0.2
$ASR (\text{Ohm cm}^2)$	Resistance at interface	20
$\sigma_{e^-} (\text{mS/cm})$	Electronic conductivity	10^{-5}
$\sigma_{M^+} (\text{mS/cm})$	Ionic conductivity	1
$L (\mu\text{m})$	SE thickness	1000

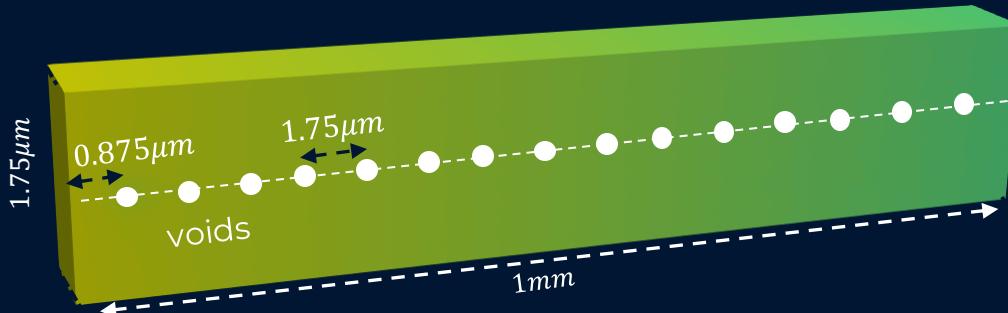
❖ Ionic current vs electronic current:



❖ Conventions

- Anode electric potential is zero: $\tilde{\mu}_{e^-}^A = 0$
- M chemical potential in metal is zero: $\tilde{\mu}_M^M = 0$

3D model shows decreasing Li deposition rate into the SE



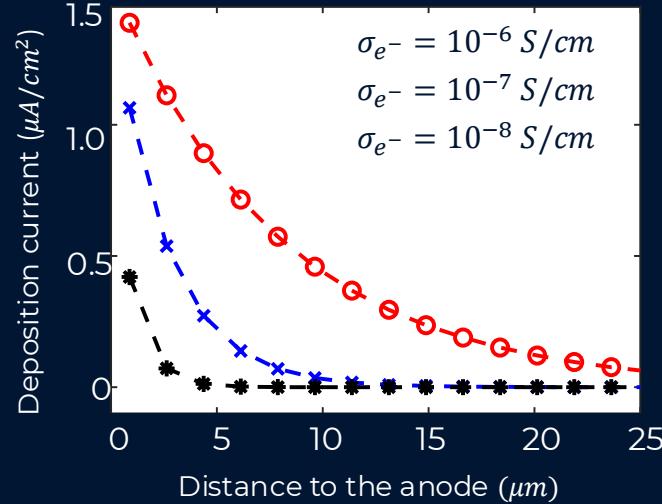
Expression	Description	Value
$i_t(\text{mA/cm}^2)$	External C.D.	0.2
$ASR (\text{Ohm cm}^2)$	Resistance at interface	20
p_{SE}	SE Porosity	5%
$r_V(\mu\text{m})$	Pore radius	0.4

- Assuming voids have same size and are evenly distributed:

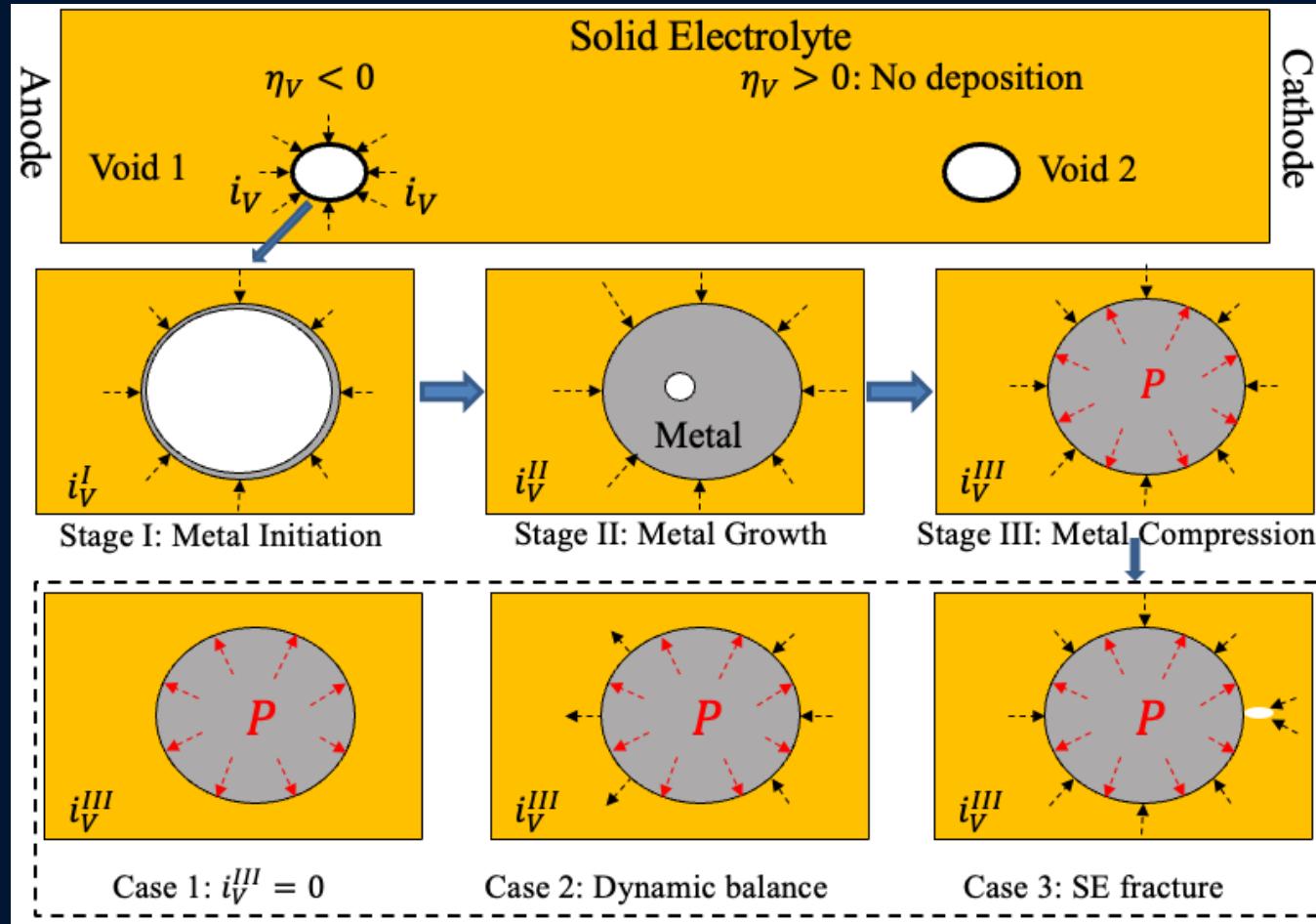
$$p_{SE} = \frac{4\pi r_V^3}{3H^3}$$

- There are 570 voids across the SE

❖ Deposition current in multiple voids inside the SE:

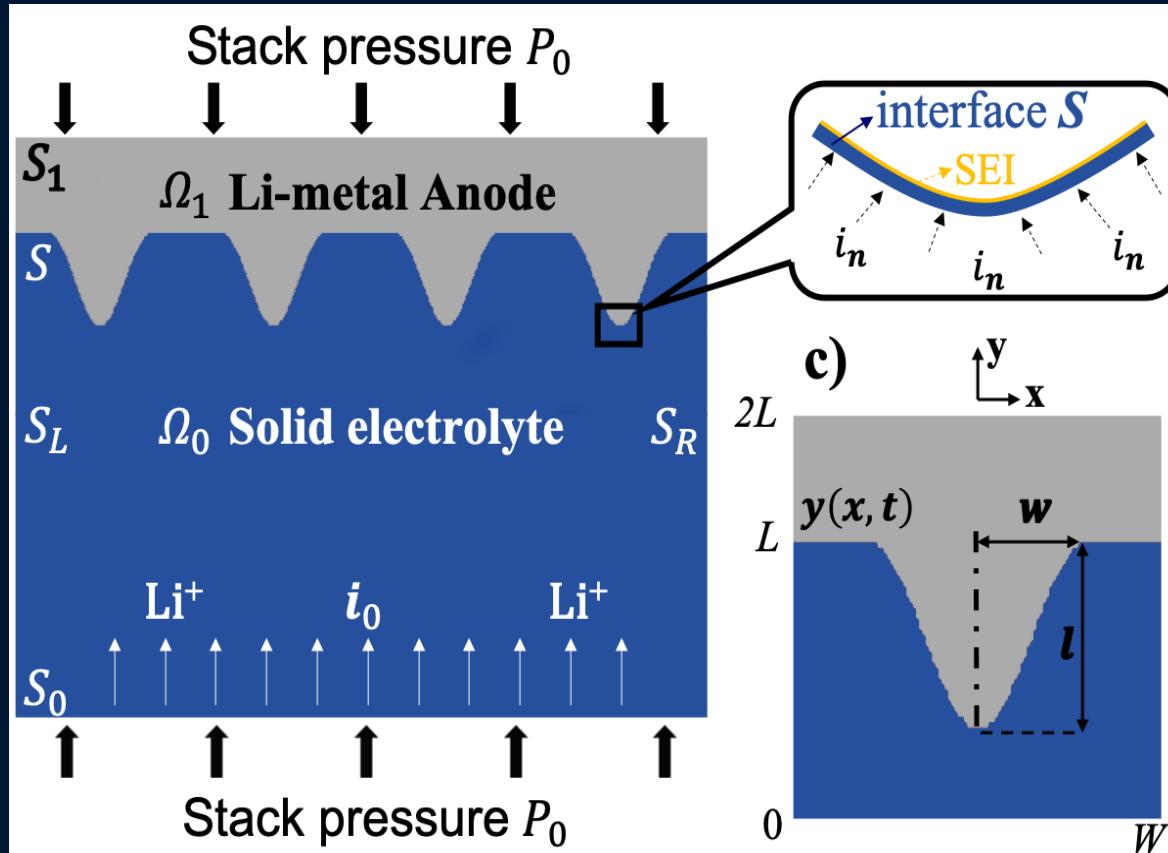


Schematics of the Li deposition in isolated voids



**Mechanism 2&1: Dendrite growth due to
electrochemistry-mechanics coupling**

Dendrite growth at the Li-metal/electrolyte interface



The ECM framework enables theory-driven research

- Butler-volmer reactions:

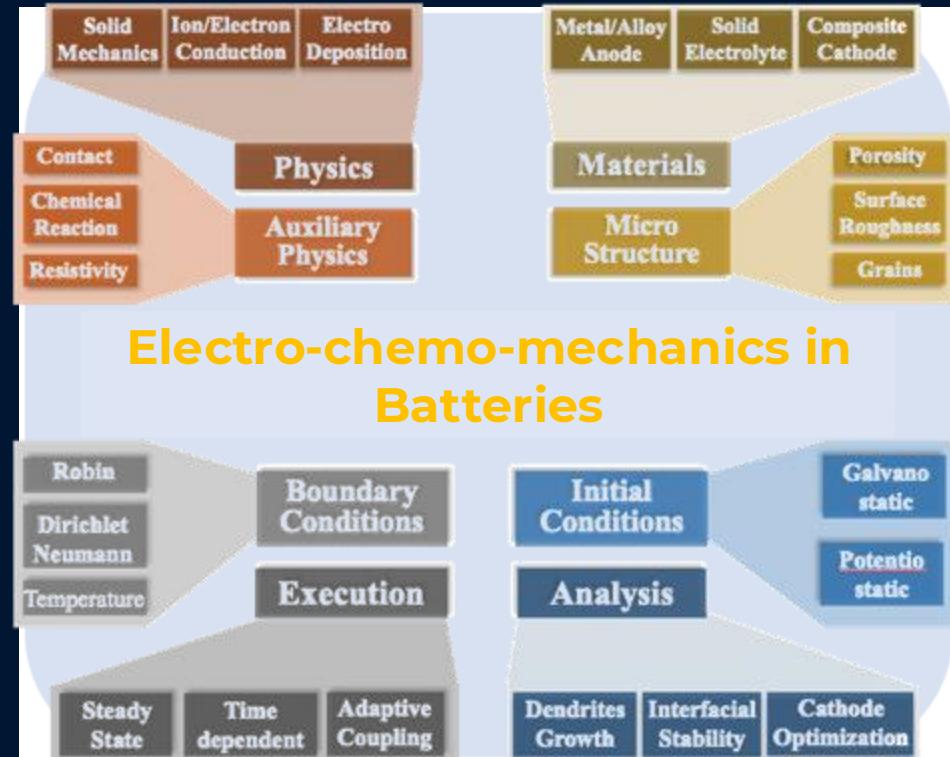
$$i_n^k = i_{exc}^k \left(e^{\frac{\alpha_a F \eta_k}{RT}} - e^{-\frac{\alpha_c F \eta_k}{RT}} \right)$$
- Diffusion in active particles:

$$\frac{\partial c_{Li}}{\partial t} = \nabla \cdot (M_{Li} \nabla \mu_{Li})$$
- Migration: $i_{M^+} = -\frac{\sigma_{M^+}}{F} \nabla \tilde{\mu}_{M^+}$
- Anisotropic volume expansion:

$$\left(\left| \frac{x}{a} \right|^{n_2} + \left| \frac{y}{b} \right|^{n_2} \right)^{n_1/n_2} + \left| \frac{z}{c} \right|^{n_1} - 1 = 0$$
- Phase segregation:

$$\mu_{Li} = \mu_{Li}^{eqm} - \nabla \cdot \left(\frac{\kappa}{\rho^2} \nabla c_{Li} \right)$$
- Electronic conduction: $i_{e^-} = \frac{\sigma_{e^-}}{F} \nabla \tilde{\mu}_{e^-}$
- Fracture in SE and cathode:

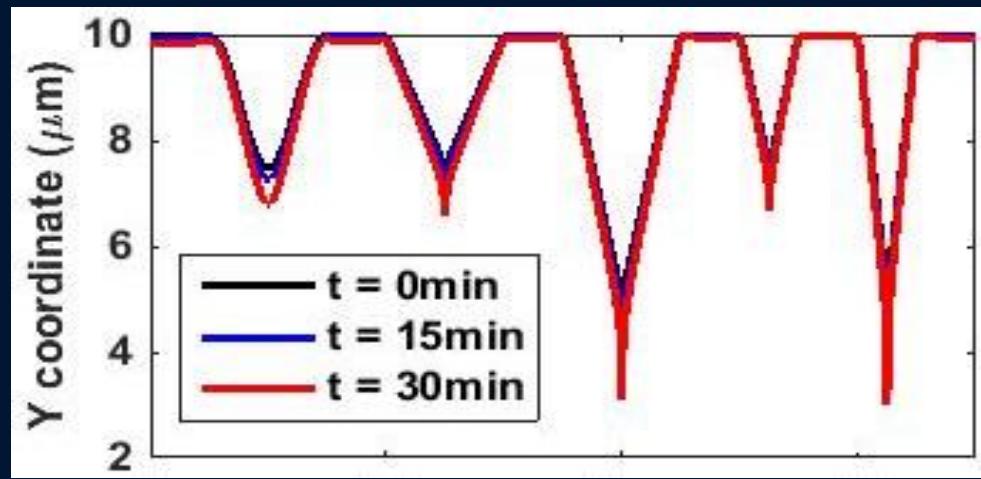
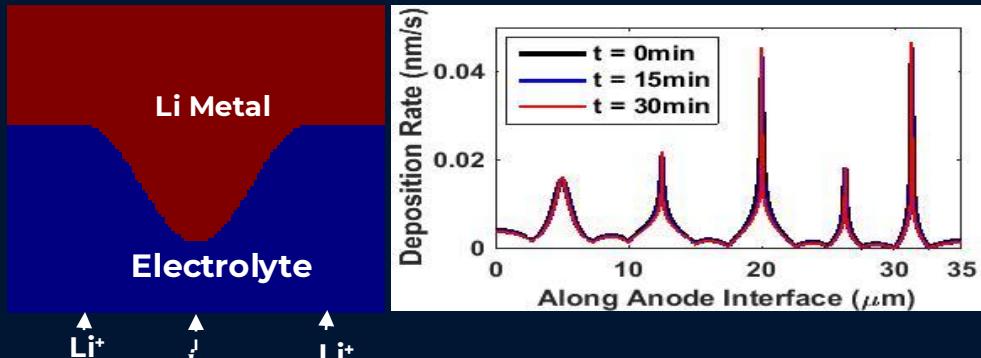
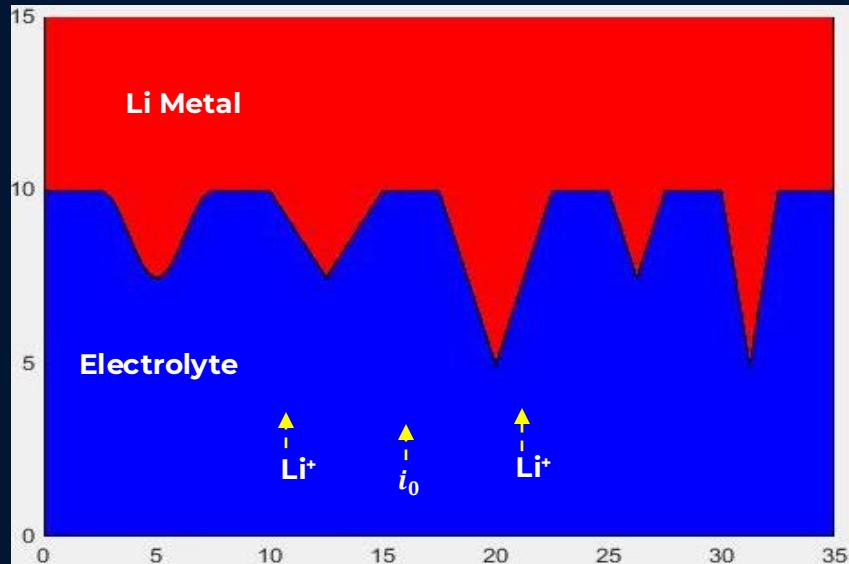
$$J = \int (W dx_2 - \mathbf{t} \cdot \frac{\partial \mathbf{u}}{\partial x_1} ds)$$
- SEI Formation: $j^{ref} = aK(c_s^{max} - c_s^{surf})^{1-\alpha} (c_s^{surf})^\alpha \left(\frac{c_l}{c_{l,ref}} \right)^{1-\alpha} [e^{\left(\frac{(1-\alpha)F\mu}{RT} \right)} - e^{\left(\frac{-\alpha F\mu}{RT} \right)}]$



Howard Tu, et al. FeEChem: An unified, open-source toolkit for modeling electro-chemo-mechanics in solid-state batteries. JMPS, Under Review.

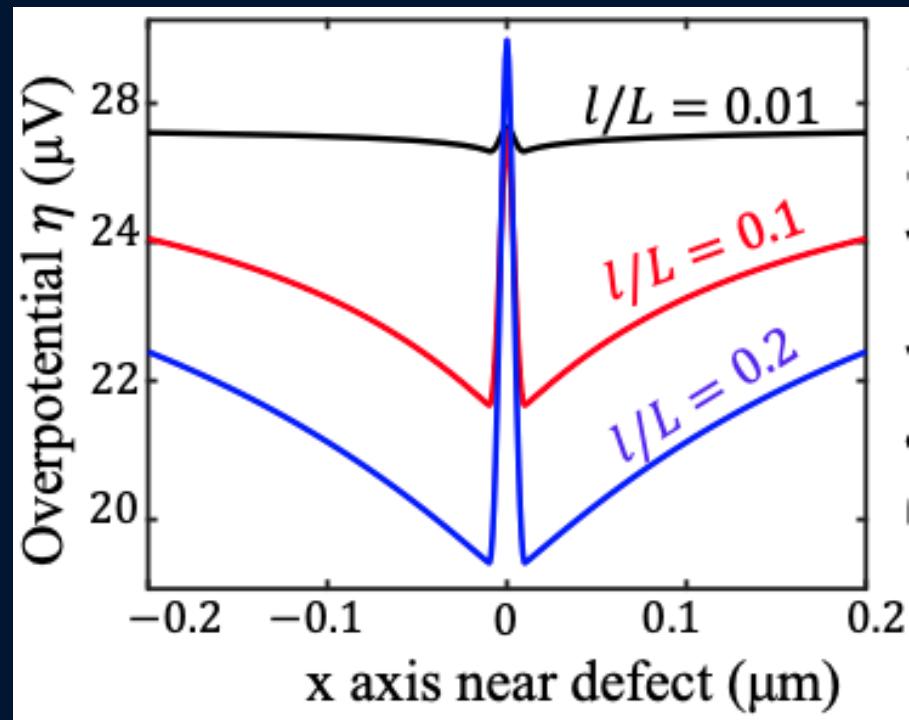
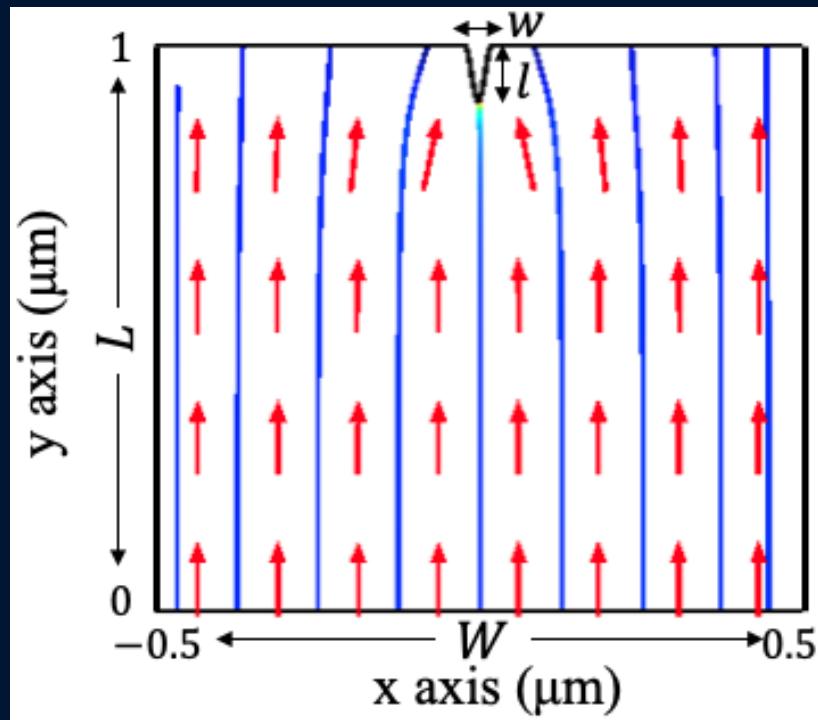
Inhomogeneous Li deposition caused by Rough Interface

System Parameters	Symbol	Value	Unit
Constant Current density	i_0	0.2	mA/cm ²
Ionic Conductivity	σ	0.5	mS/cm
Equilibrium Potential	E_{eq}	0	V
Anode Voltage	E_{anode}	0	V

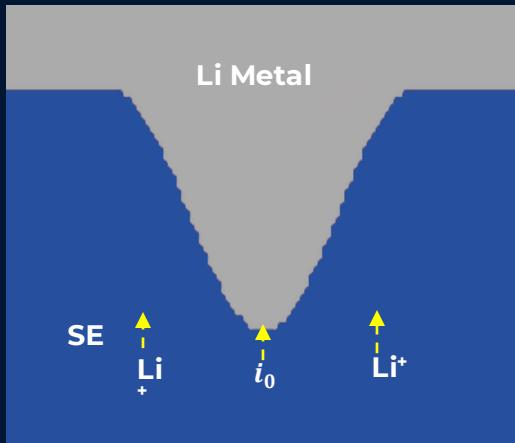


Inhomogeneous current & Overpotential at the Li metal/SE interface is affected by roughness

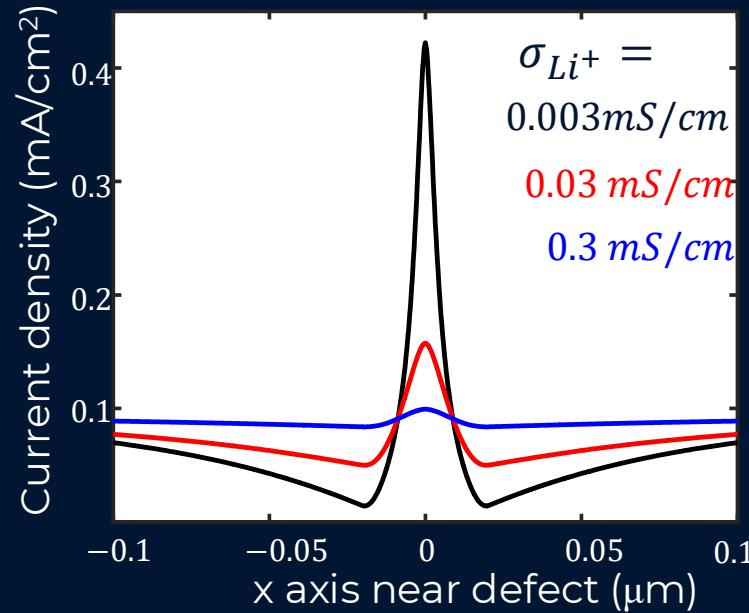
- ❖ Current density concentrates near the defect between Li metal and the SE.
- ❖ Surface overpotential is inhomogeneous as defect (l/L) grows larger.



Higher ionic conductivity will reduce deposition inhomogeneity

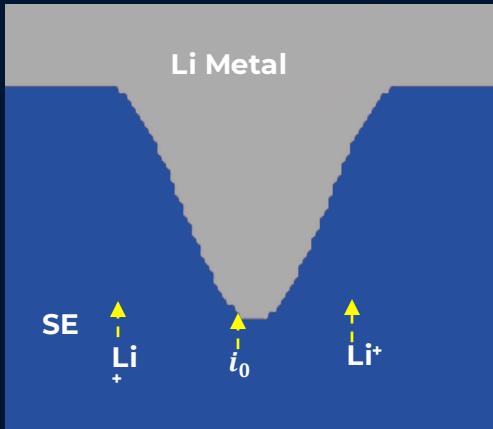


Expression	Description	Value
$ASR(\Omega \text{ cm}^2)$	Area-specific-resistance	12.5
σ_{Li^+} (mS/cm)	Ionic conductivity	Vary
$i_0(\text{mA}/\text{cm}^2)$	Applied C.D.	1
$L (\mu\text{m})$	SE thickness	1000
$w (\mu\text{m})$	Width of defect	1
$l (\mu\text{m})$	Length of defect	20

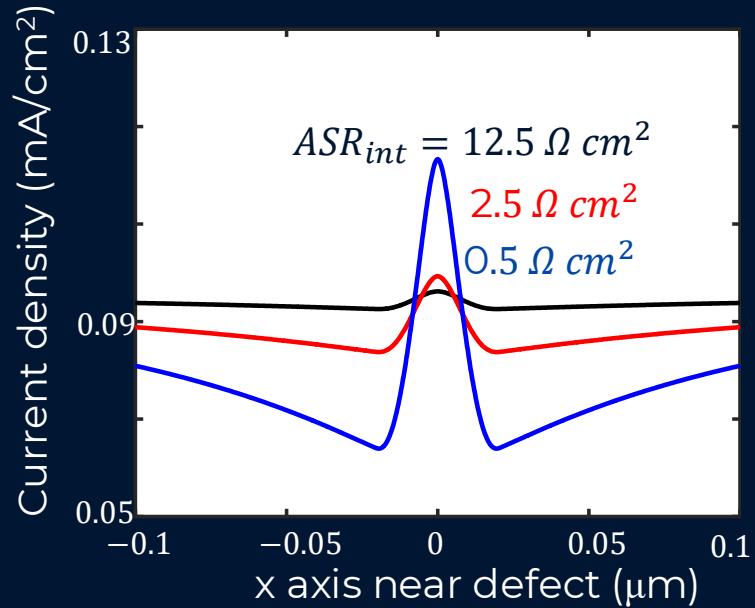


- Current density becomes more even as ionic conduction in SE is faster (σ_{Li^+} is larger).
- σ_{Li^+} is always good when getting larger

Lower interfacial area-specific-resistance (ASR) cause higher deposition inhomogeneity



Expression	Description	Value
$ASR(\Omega \text{ cm}^2)$	Area-specific-resistance	vary
σ_{Li^+} (mS/cm)	Ionic conductivity	0.3
$i_0(\text{mA}/\text{cm}^2)$	Applied C.D.	1
$L (\mu\text{m})$	SE thickness	1000
$w (\mu\text{m})$	Width of defect	1
$l (\mu\text{m})$	Length of defect	20

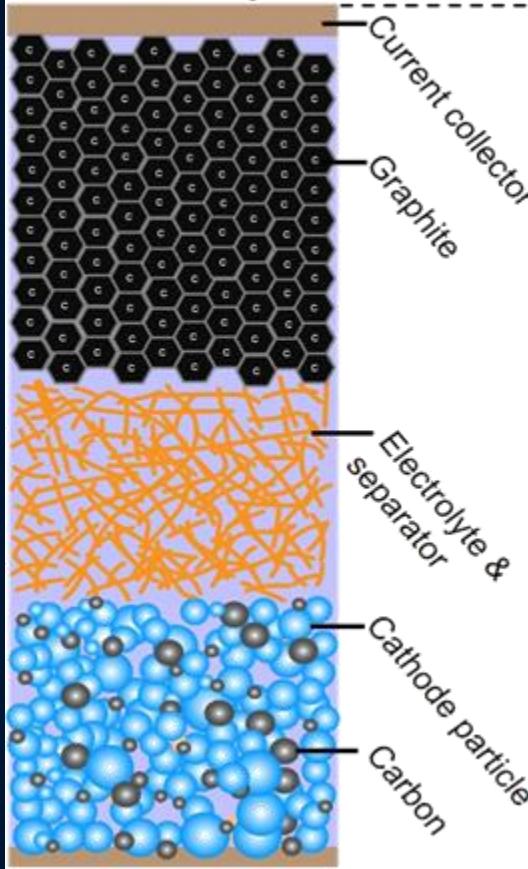


- Current density becomes more evenly distributed as the charge transfer reaction is slower (ASR is larger).
- ASR is not always good when getting too small

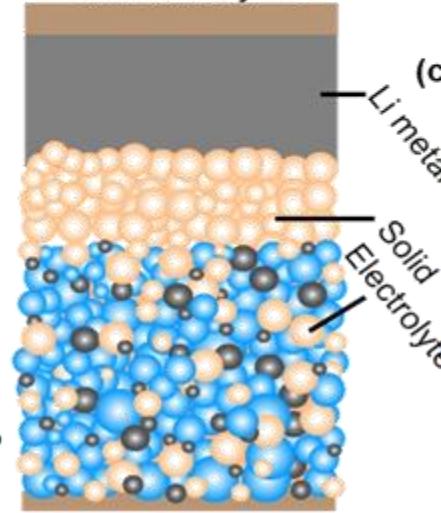
Anode-free Batteries as solution for dendrite issues

The roadmap for anode-free batteries

(a) Conventional Li-ion battery

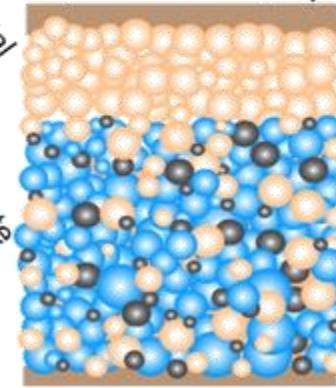


(b) Li-metal solid-state battery



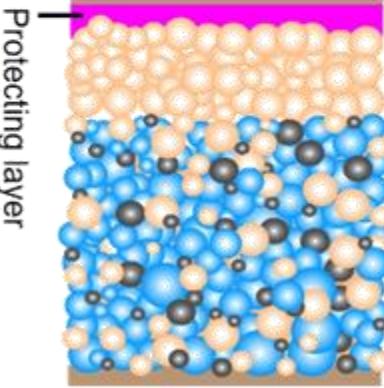
~50 %

(c) Anode-free solid-state battery



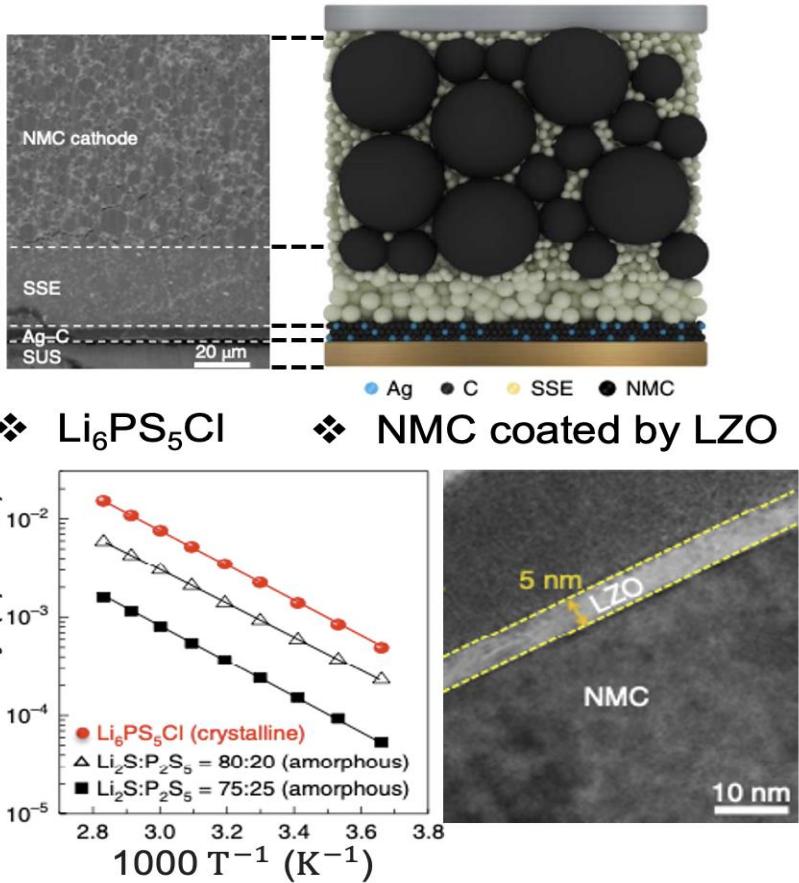
~62 %

(d) Anode-free solid-state battery with a protecting layer

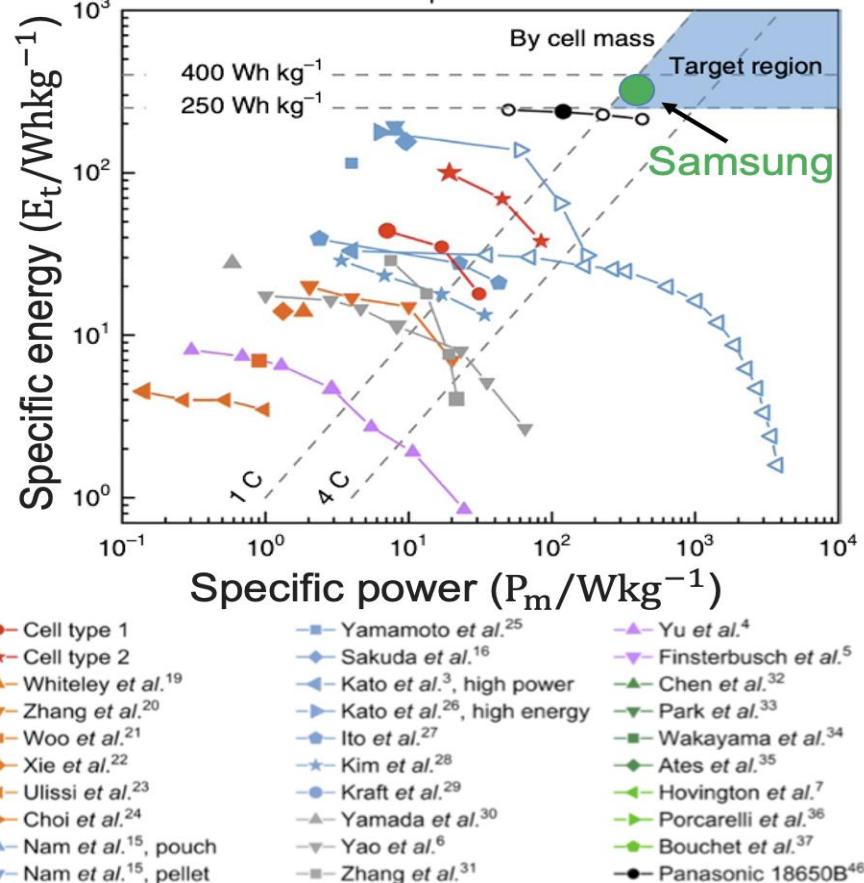


~59 %

Successful trial from Samsung on AgC interlayer



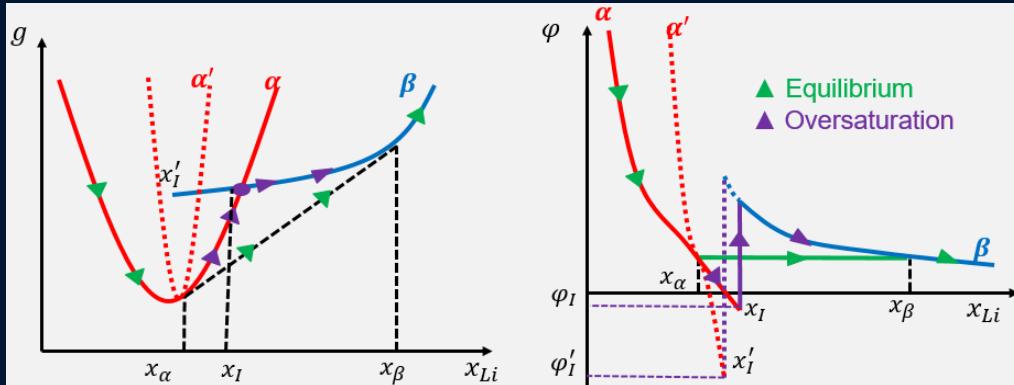
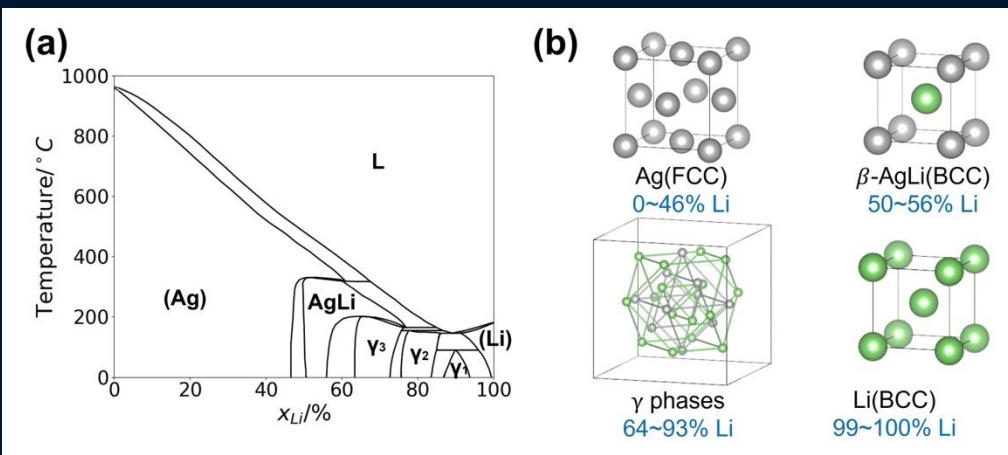
Lee, Yong-Gun, et al. *Nature Energy* 5.4 (2020): 299-308.



Randau, Simon, et al. *Nature Energy* 5.3 (2020): 259-270.

Why Ag is good? Reason 1: Wider phases enable smoother oversaturation

- First-principle calculations on Li-metal alloy



Flatter free energy curves leads to:

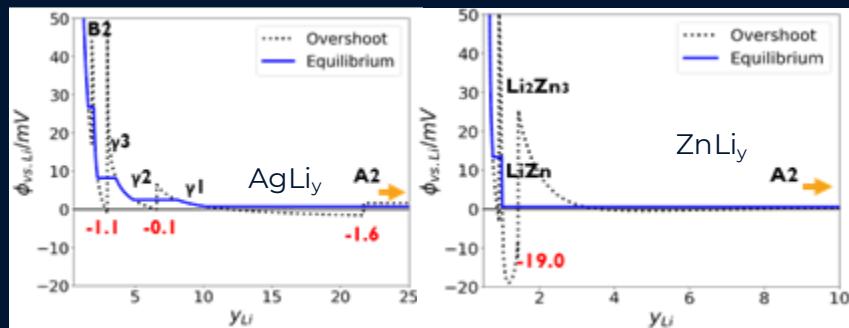
- Less voltage drop at Li over-saturation
- Continuous lithiation
- Prevents Li deposition elsewhere (carbon-SE interface, etc.)



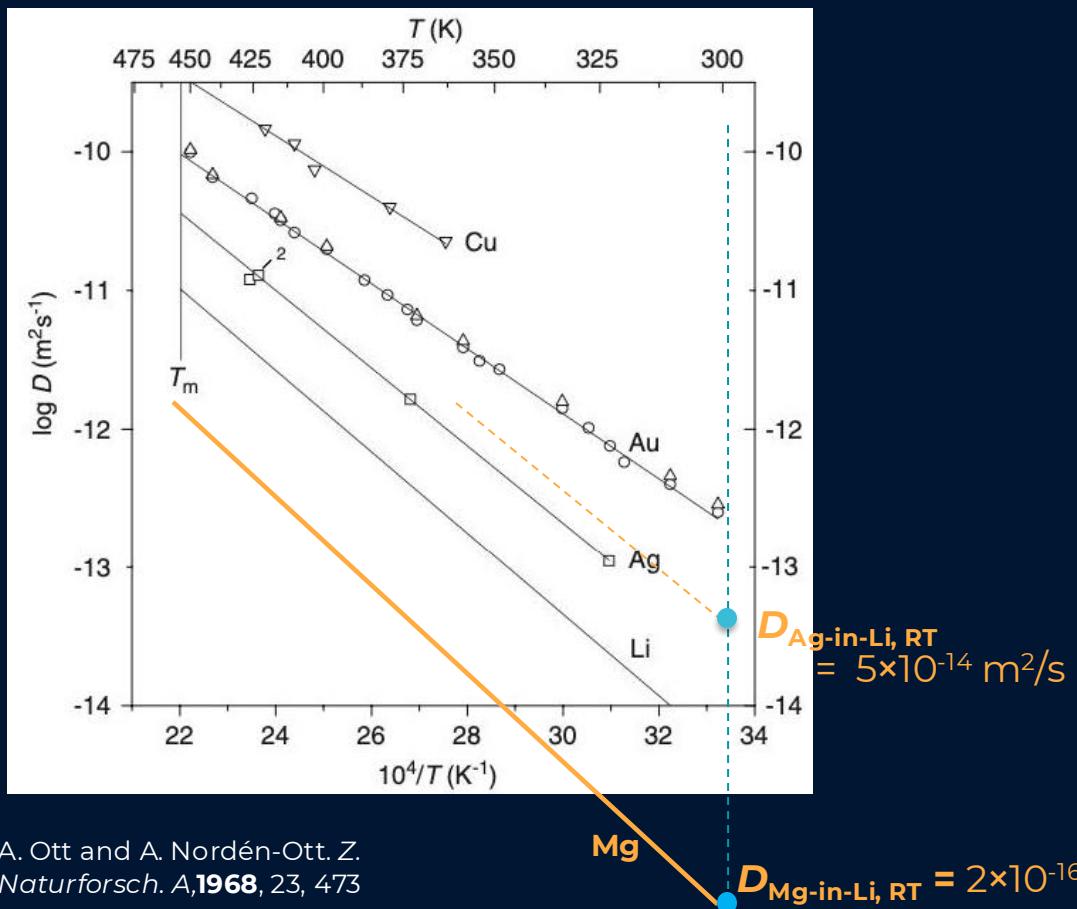
Ag:

- Very low over-potential
- Continues absorbing Li

Other metals (Zn, Sn, Ni, etc.):
High overpotential upon compound formation
Further lithiation prohibited

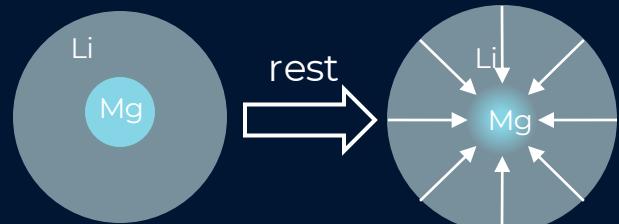


Why Ag is good? Reason 2: Rapid Ag Diffusion in Li phase



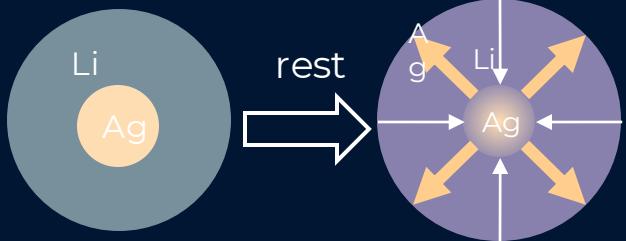
Slow Mg diffusion

$$D_{\text{Mg-in-Li, RT}} = 2 \times 10^{-16} \text{ m}^2/\text{s}$$



Rapid Ag diffusion

$$D_{\text{Ag-in-Li, RT}} = 5 \times 10^{-14} \text{ m}^2/\text{s}$$



Why Ag is good? Reason 3: Large volumetric increase during alloying

Volume expansion ratio of alloys at room temperature suppose lithiation stops at the last phase before reaching BCC-Li (A3)

Metal	last phase	Max x_{Li} in P	R
Ag	γ_1	0.94	17.7
Au	$\text{Au}_4\text{Li}_{15}$	0.789	4.7
Zn	ZnLi	0.5	2.0
Sn	$\text{Sn}_4\text{Li}_{17}$	0.809	3.6
Al	Al_4Li_9	0.692	3.4
Cu	(Cu)	~0.25	1.4
Ni	(Ni)	~0	~1
Si	$\text{Si}_4\text{Li}_{17}$	0.809	4.1

$$R = \frac{\text{Volume per atom in alloy}}{\text{Volume per atom in metal}} \times \frac{1}{1 - x_{\text{Li}}}$$

Metal	last phase	Max x_{Li} in P	R
Bi	BiLi_3	0.75	2.1
Pt (?)	PtLi_2 (PtLi_5 ?)	0.667 (0.833?)	1.8? (~6?)
Ga	GaLi_2	0.667	2.4
Ge	$\text{Ge}_4\text{Li}_{17}$	0.809	3.7
Pb	$\text{Pb}_4\text{Li}_{17}$	0.809	3.2
Tl	$\text{Tl}_5\text{Li}_{22}$	0.815	3.5
Sb	SbLi_3	0.75	2.3
In	$\text{In}_3\text{Li}_{13}$	0.8125	4.0

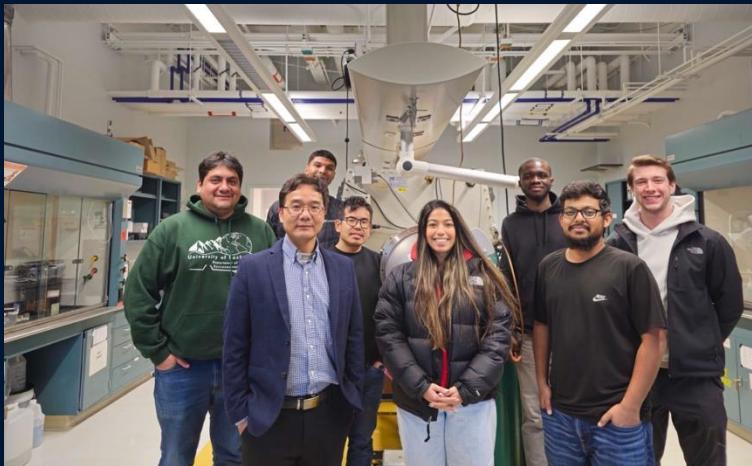
- Ag is the only metal in the table with significant volume expansion to extrude
- Mg might also reach large volume expansion because of high inter-solubility with Li

Summary

1. Dendrite issues in solid-state batteries are a multiscale problem.
 2. Multiscale modeling from atomic to continuum scale is needed.
 3. Machine learning has the potential to link all scales together.
-

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❖ RIT's battery center



❖ Funding support



Seedling grant



SAMSUNG
ADVANCED
INSTITUTE OF TECHNOLOGY



THANK YOU!

Q&A

Do you have any questions?

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Rochester Institute of Technology

