# Towards an Optimized Composite Cathode Structure (WP2)

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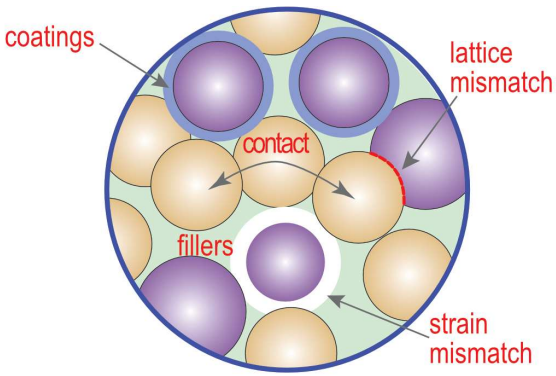
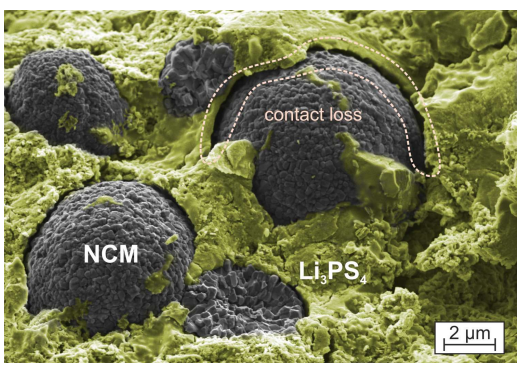
SOLBAT

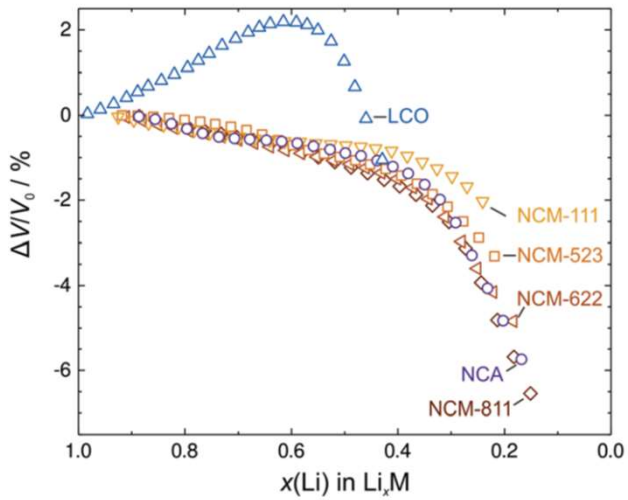
# Motivation: mechanical degradation




*Koerver et al. Chem.Mater. 29 (2017)*

- Large volume change of active material




- Stiff and brittle nature of solid electrolyte/cathode material

| Solid Electrolyte | Young's modulus | Fracture toughness |
|---|---|---|
| LLTO | ~200GPa | ~1MPa $m^{1/2}$ |
| LLZO | ~150GPa | |
| LAGP | ~115GPa | |
| LPS | ~20GPa | ~0.23MPa $m^{1/2}$ |

| Cathode Material | Young's modulus | Fracture toughness |
|---|---|---|
| LCO | ~190GPa | ~0.9MPa $m^{1/2}$ |
| NMC | ~200GPa | ~0.3MPa $m^{1/2}$ |
| LMO | ~194GPa | ~0.5MPa $m^{1/2}$ |

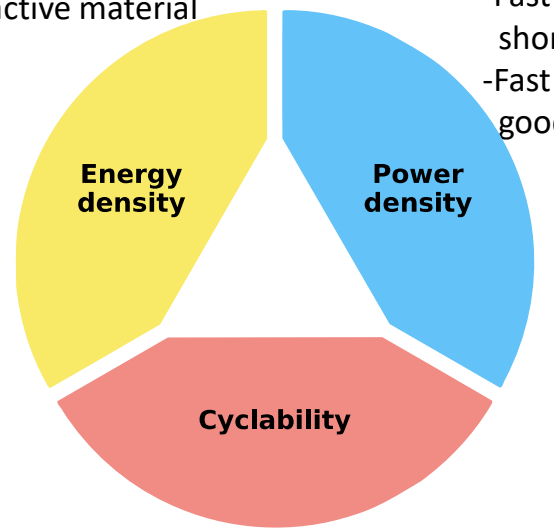
*Wolfenstine et al. Ionics 24 (2018), McGrogan et al. Adv.Energy Mat. 7 (2017), Xu et al. JES 164 (2017), Koerver et al. EES 11 (2018)*

Can we make the cathode more compliant?

Can we suppress the cathode volume expansion?

# Motivation: composite structure

-Large volume fraction of active material

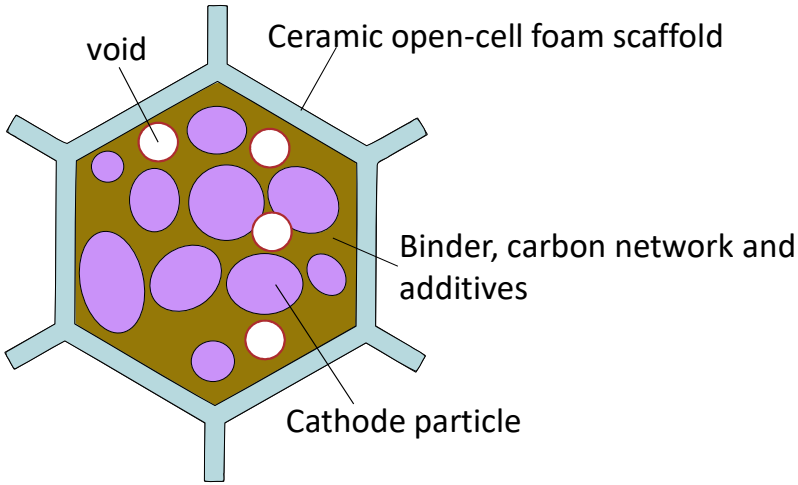



-Fast reaction:
large surfaces of active material
-Fast Li-ion transport:
short Li-ion pathway
-Fast electron transport:
good electronic conductivity

-Good mechanical integrity:
no delamination and fracture during cycling

We propose a composite cathode, which has

- solid ceramic electrolyte open-cell foam scaffold
- carbon network interpenetrating the ceramic electrolyte
- cathode particles filling gaps between the two networks




We can optimise TOPOLOGY and POROSITY to accommodate swelling

# Structured material: increased compliance

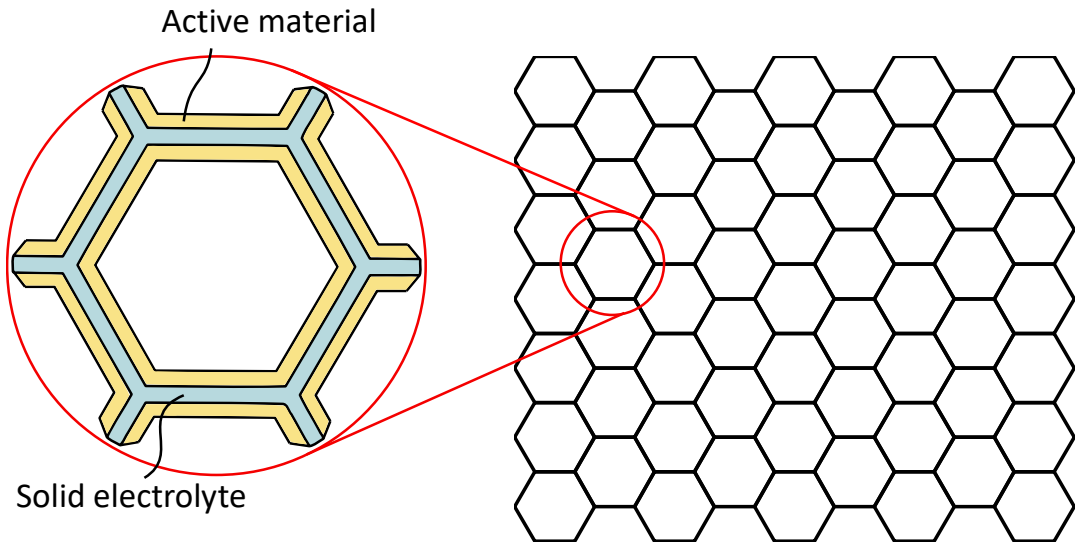
Young's modulus:

$$E^{\infty} \sim E_s \bar{\rho}_s^3$$

Bulk modulus (perfect):

$$K^{\infty} \sim K_s \bar{\rho}_s$$

$\bar{\rho}_s, E_s, K_s$ – Volume fraction, Young's modulus and bulk modulus of solid




By increasing porosity, the elastic moduli can decrease significantly ($\sim\bar{\rho}^3$) , thus increasing the compliance

# Structured material: increased compliance

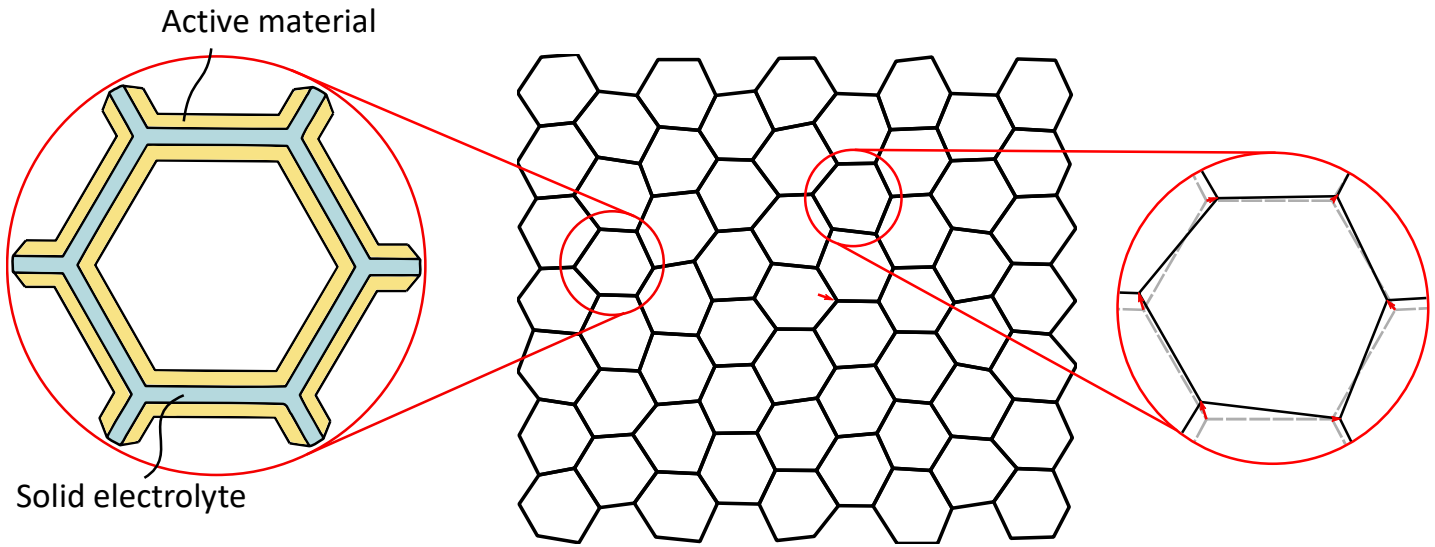
Young's modulus:

$$E^{\infty} \sim E_s \bar{\rho}_s^3$$

Bulk modulus (distorted):

$$K^{\infty} \sim K_s \bar{\rho}_s^3$$

$\bar{\rho}_s, E_s, K_s$ – Volume fraction, Young's modulus and bulk modulus of solid

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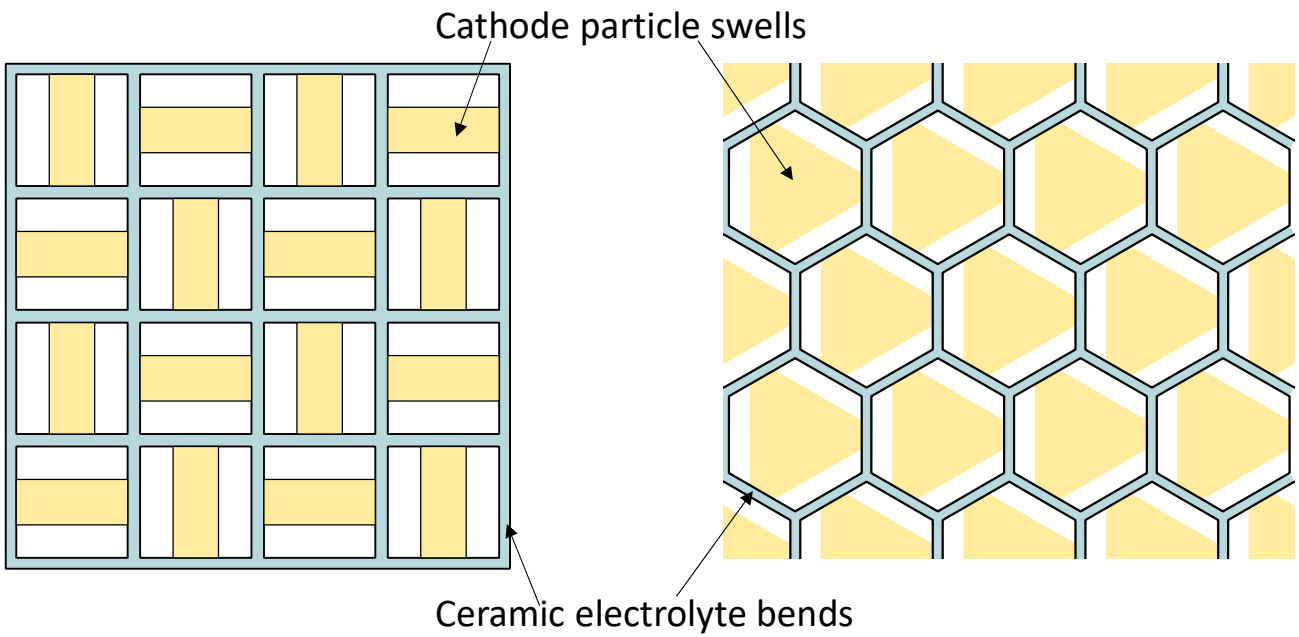
# Structured material:
# zero macroscopic strain upon simultaneous expansion of active material

We may borrow the idea of zero Coefficient of Thermal Expansion (CTE): by combining two materials with different CTE, we can achieve zero thermal expansion of the composite structure upon temperature change.




And **local strain** in electrolyte less than actuation strain by a factor of $\bar{\rho}_{se}$

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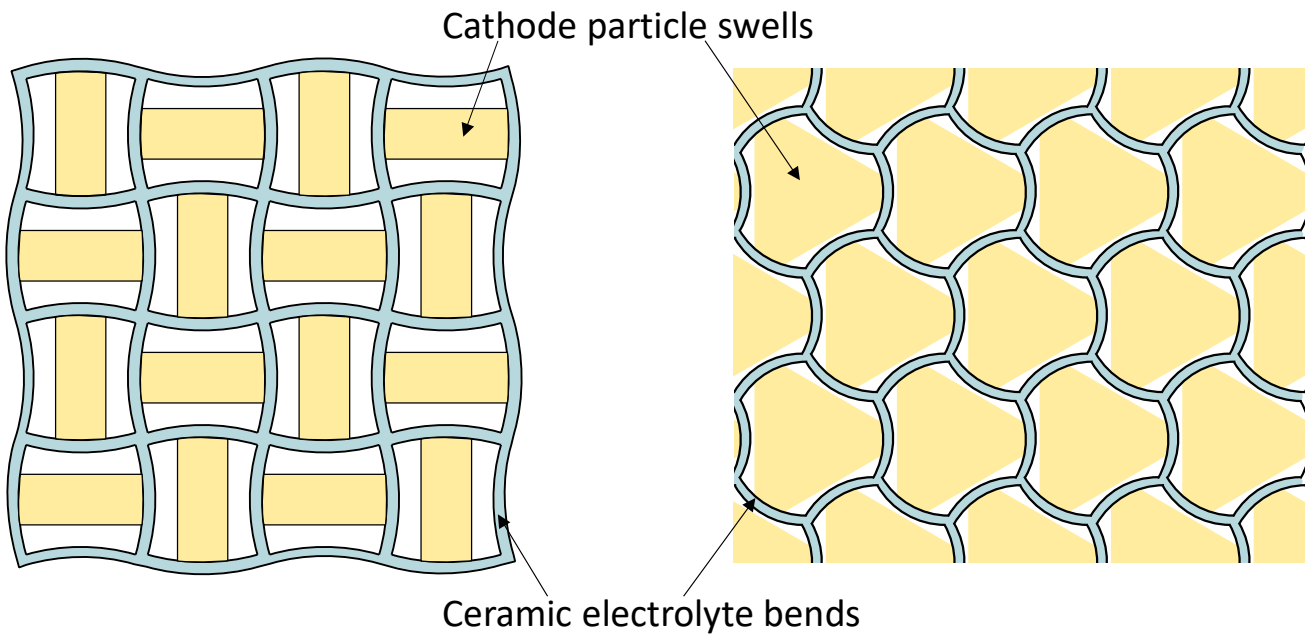


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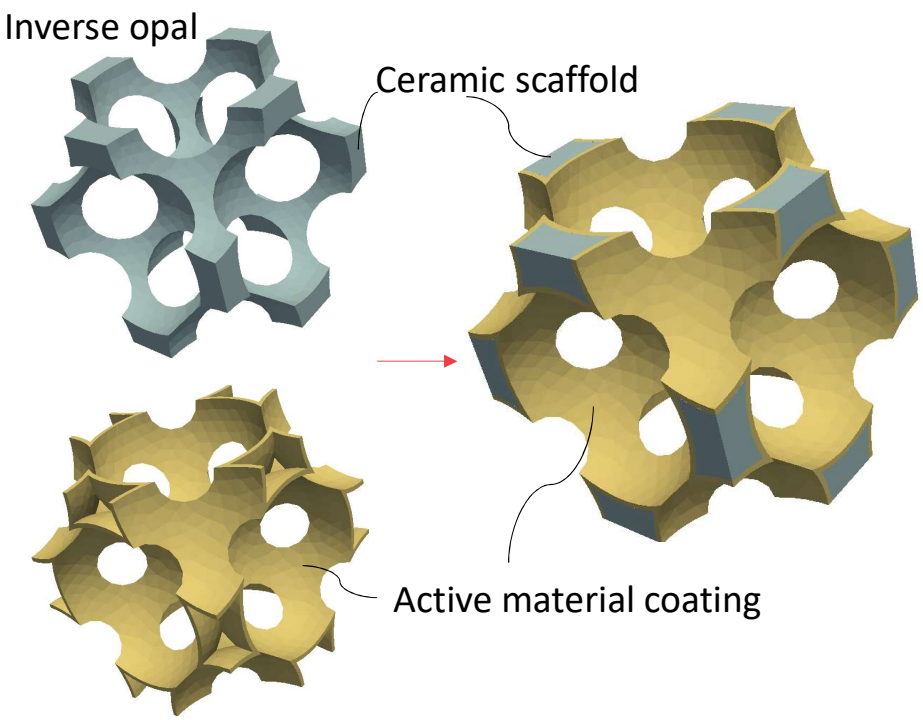
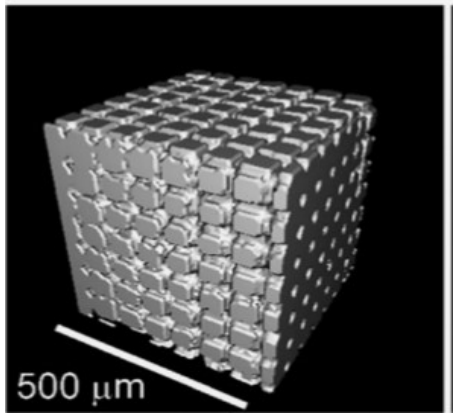
# Engineering the material: scalability?




3D printing




Tape casting

*Zekoll et al. EES 11 (2018, Fu teal. EES 10, (2017))*

Thanks!