NUMAP-FOAM Summer School 2023

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ACoM | RWTH Aachen University | Forschungszentrum Jülich (IEK-2)

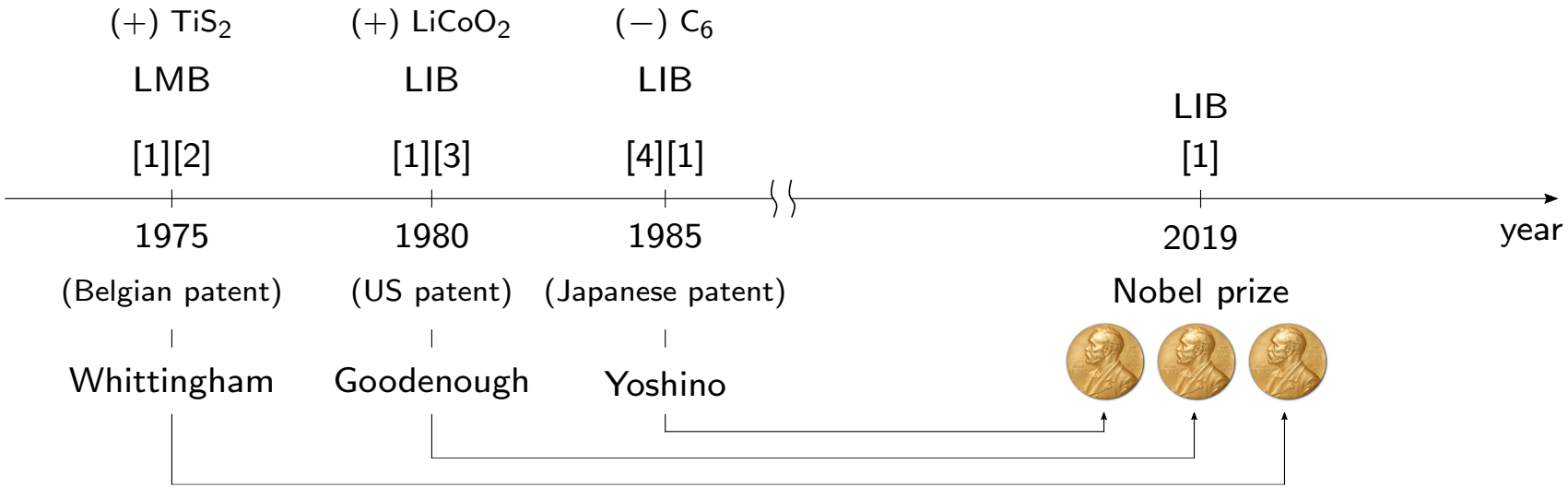
Applied and Computational Mathematics

RWTH AACHEN UNIVERSITY

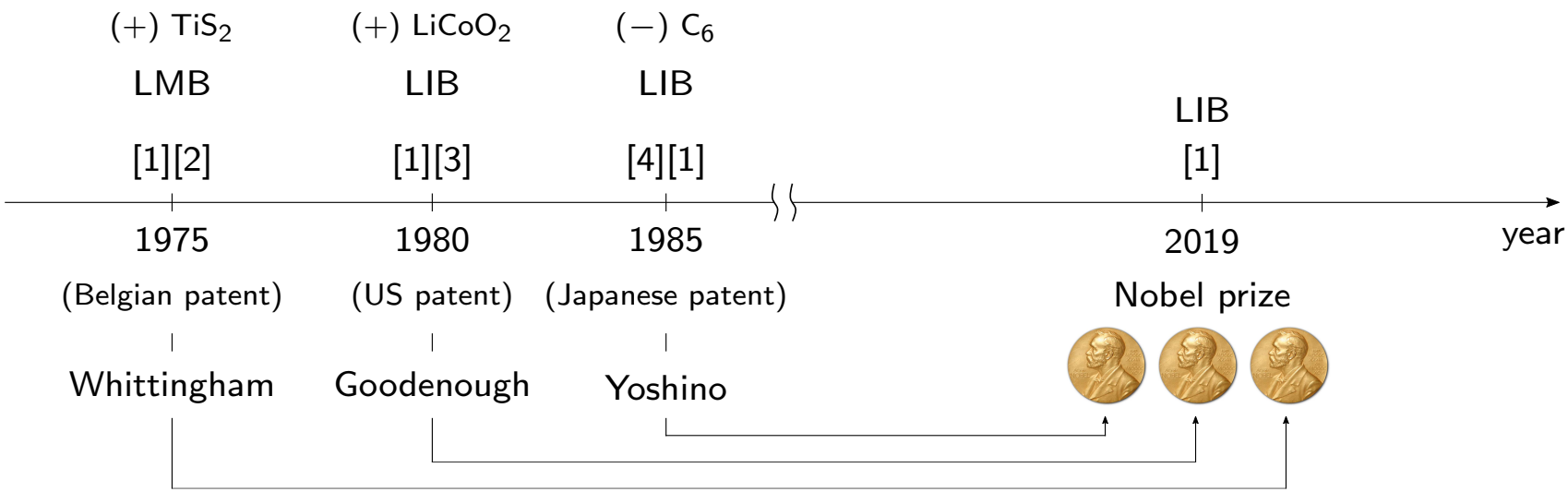
Cambridge, 04 September 2023

Content

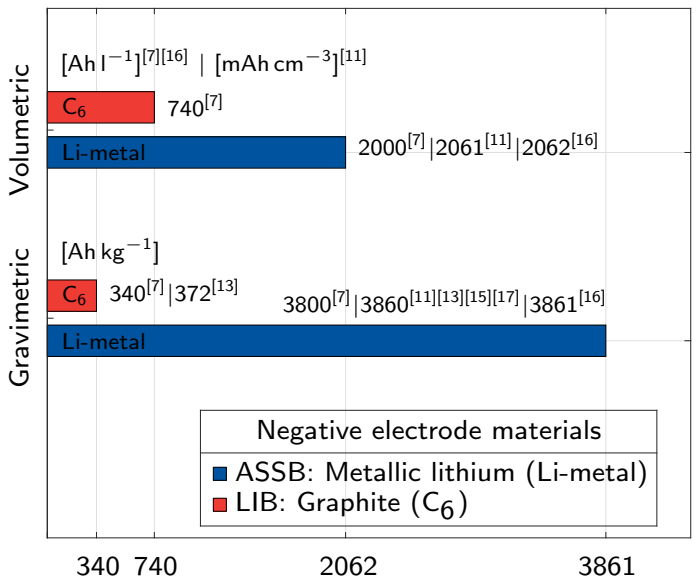
(i) Motivations: Rechargeable Lithium-ion battery (LIB)



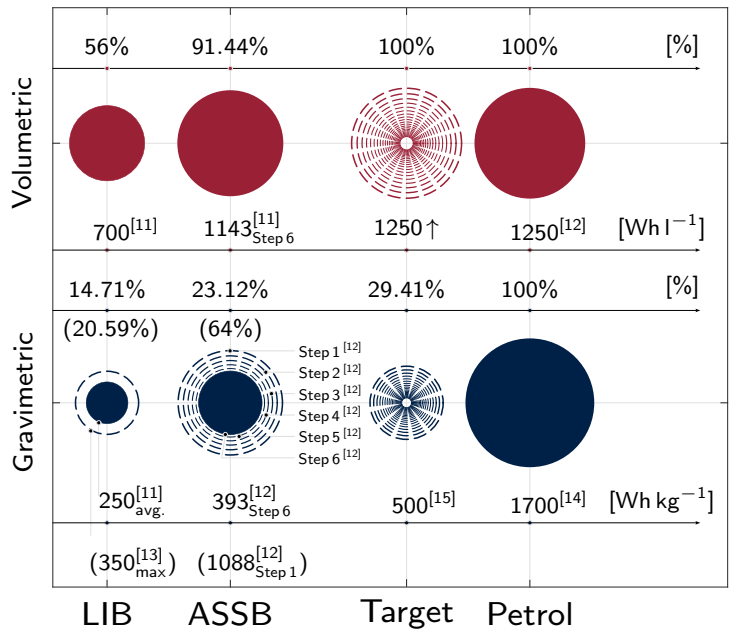
(i) Motivations: LIB → limits



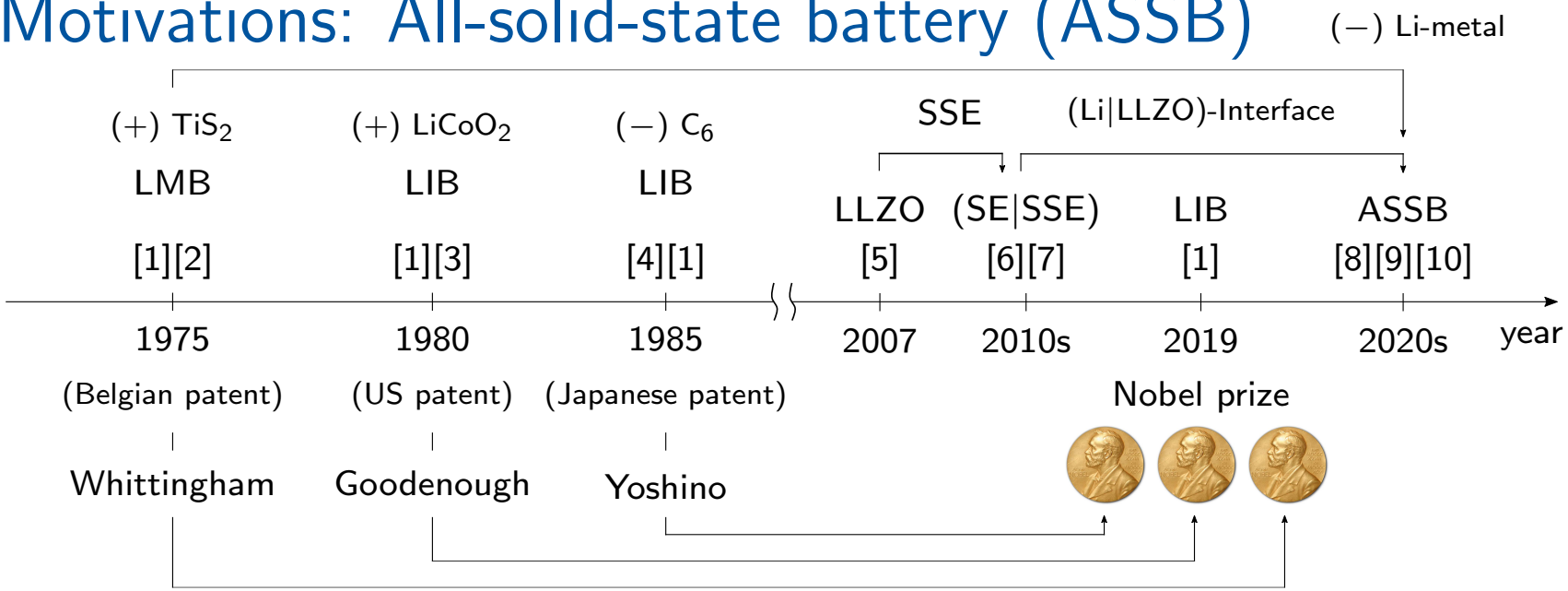
Theoretical capacity of charge:
pure metallic lithium (Li-metal) versus Graphite (C_6)



Energy density: ASSB versus LIB versus Petrol



(i) Motivations: All-solid-state battery (ASSB)



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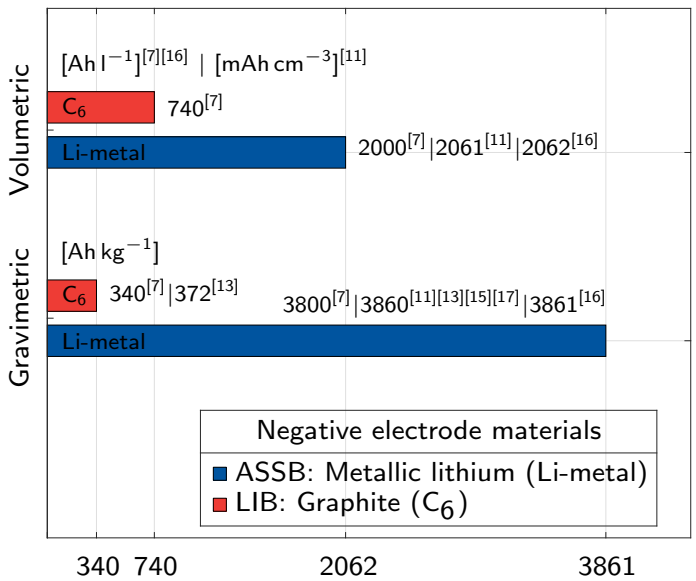

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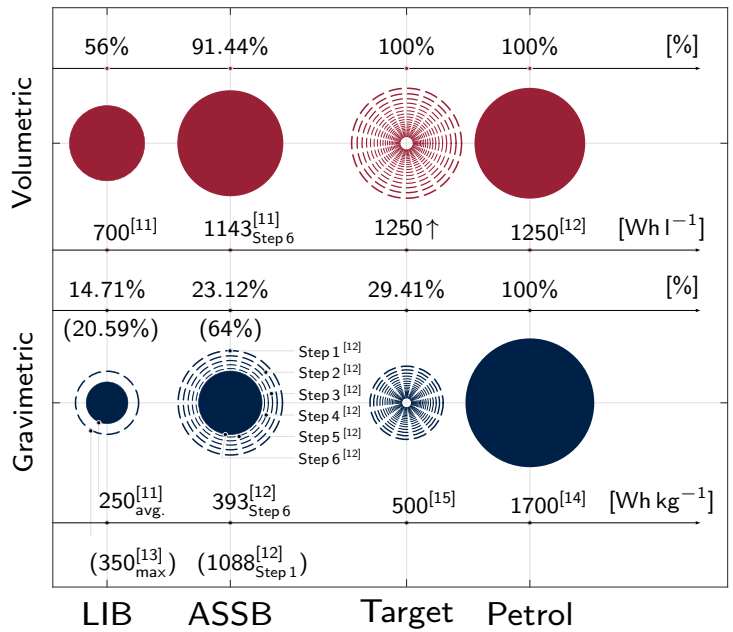
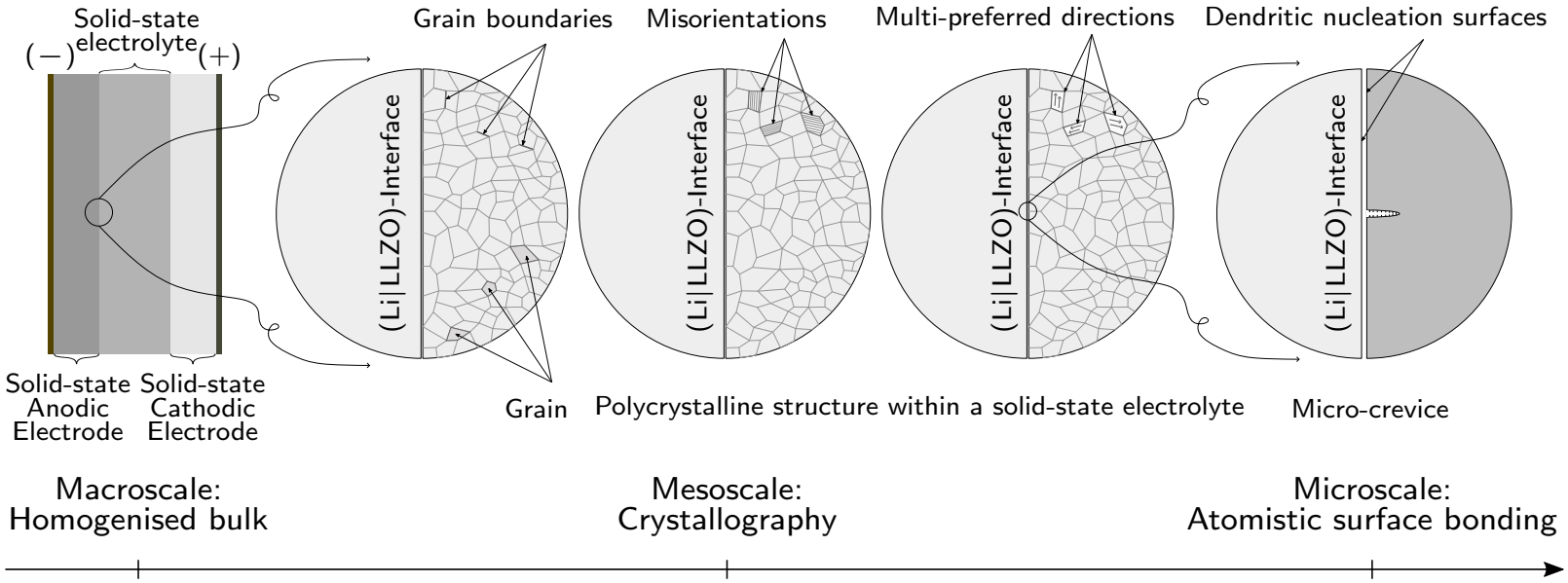


(ii) PhD Project: Interface analysis and numerical modelling



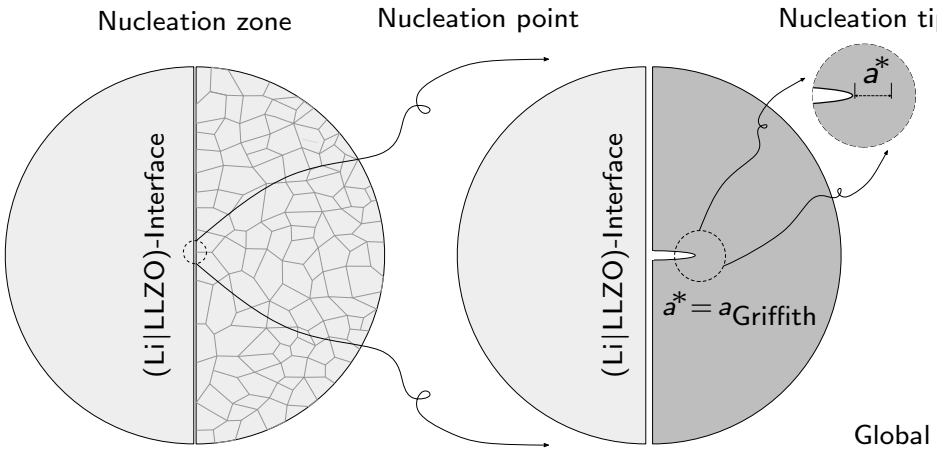
Find a such that the following coupled problem $\forall\, a \in \mathcal{V}$ hold:

$$\rho \frac{\partial \boldsymbol{U}}{\partial t} - \nabla \cdot \left(\mathbb{C}^{T_f \phi}_{(\lambda,\mu)} : \nabla \boldsymbol{U}^{(s)} \right) + \rho \nabla V_E = \mathbf{0}, \tag{1}$$

$$\text{s.t.} \quad a_{\text{Griffith}} := a^* = \arg\min_{a \in \mathcal{V}} \left\{ \iiint_{\Omega} f(a, \boldsymbol{u}, \theta, c^{m|\text{Li}^+|n}; \lambda, \mu, \boldsymbol{d}_{G_j} \otimes \boldsymbol{d}_{G_j})\, d\Omega \right.$$

$$\left. - \iint_{\Gamma} f(a; \gamma)\, d\Gamma \right\} \tag{2}$$

(ii) PhD Project: Interface analysis and numerical modelling

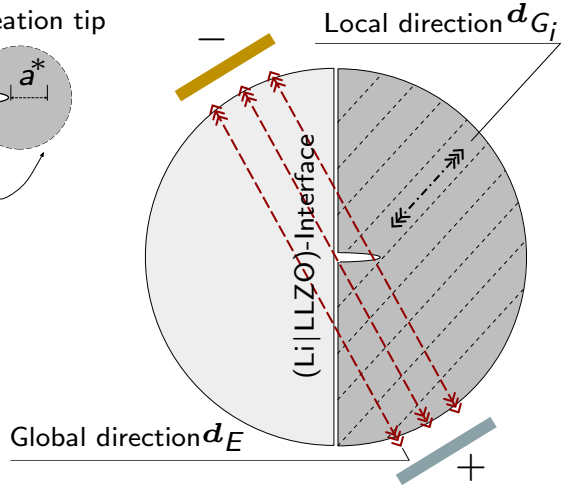


SCL

Dendrite growth

Griffith criterion a^*

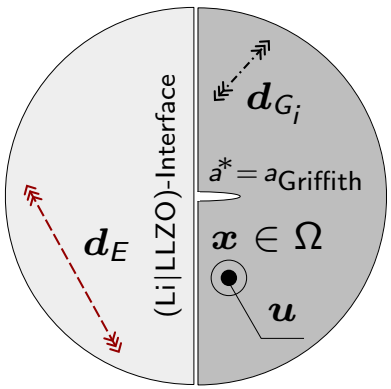
Cracking nucleation



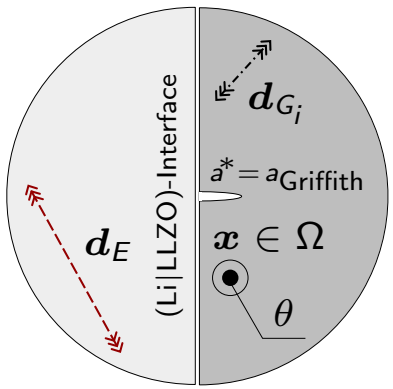
Misorientation $\boldsymbol{M} = \boldsymbol{d} \otimes \boldsymbol{d}$

Global direction: Uniform electric field $\boldsymbol{d}_E$

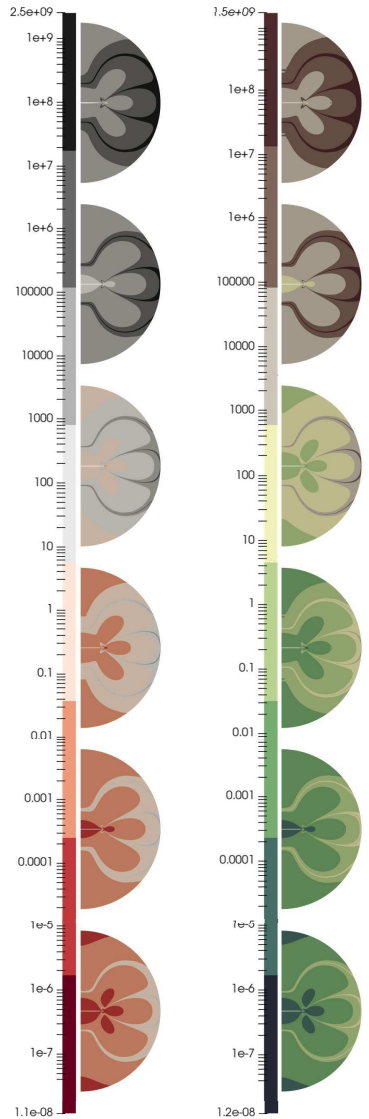
Local direction: Crystallographical orientation $\boldsymbol{d}_{G_i}$



Displacement field $\boldsymbol{u}$

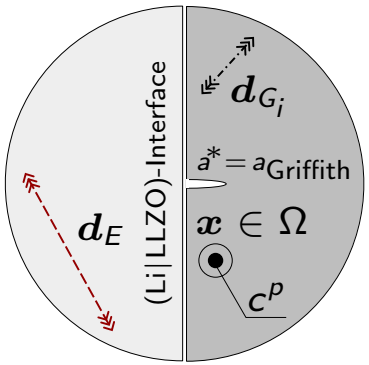


Temperature field θ

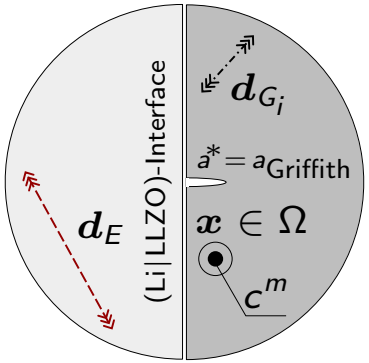


(iii) Looking forward at NUMAP-FOAM Summer School:

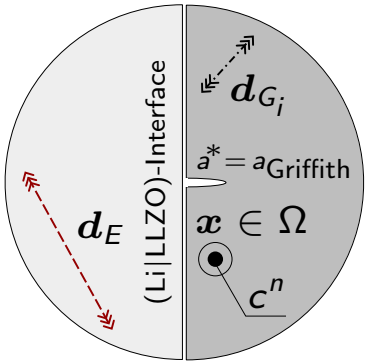
1. Compute and visualise the transport of Li-ions, Anions, Vacancies hopping at the critical (Li|LLZO)-Interface.



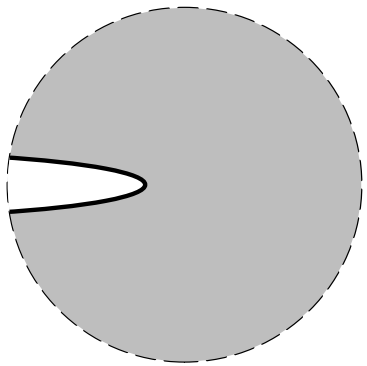
Cation Li^+concentration field c^p



Anion concentration field c^m



Vacancy concentration field c^n



Boundary condition around pre-existing crevice open at (Li|LLZO)-Interface

2. Learning skills, comments, tips & tricks about FOAM.
3. Extending networks and connections.

Thank you for your listening.