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Modeling and simulations towards high performance batteries

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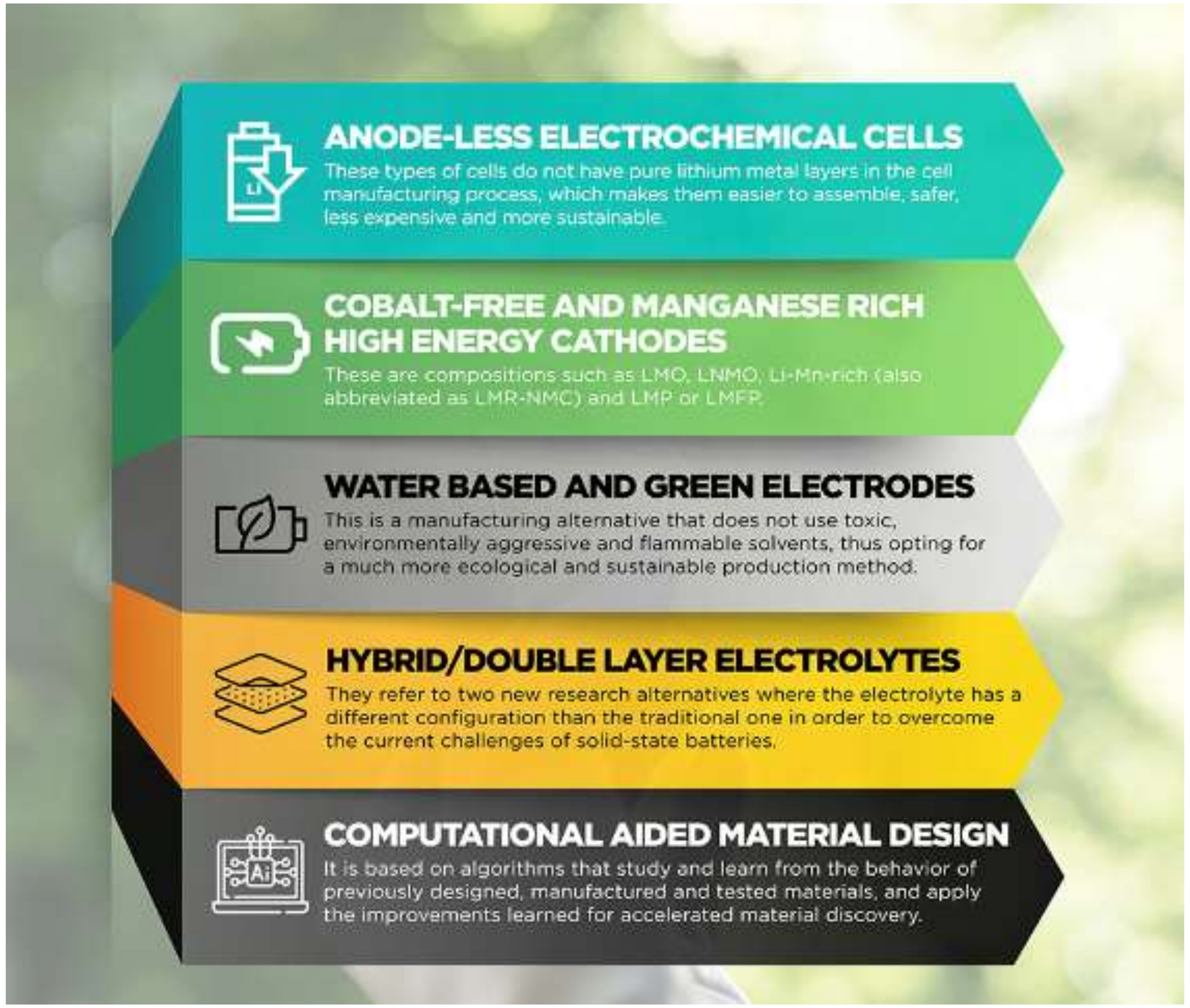
IL RICICLO DELLE BATTERIE AL LITIO. Innovazione in ambito di economia circolare applicata al recupero di metalli strategici

C S M T

30.03.2023

5 key concept that will shape electrochemistry in 2023



by CIC energiGUNE

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Multiscale Mechanics and Multiphysics of Materials Lab

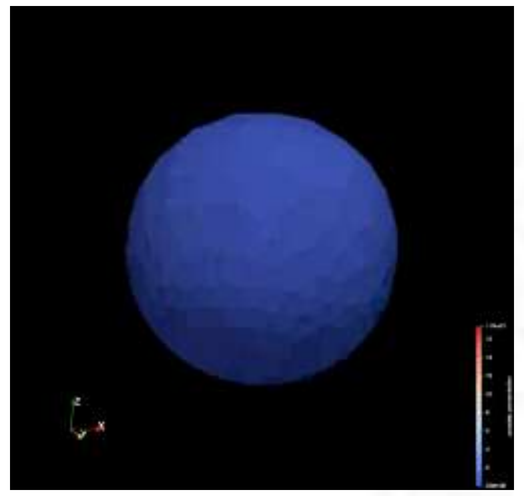
https://m4lab.unibs.it

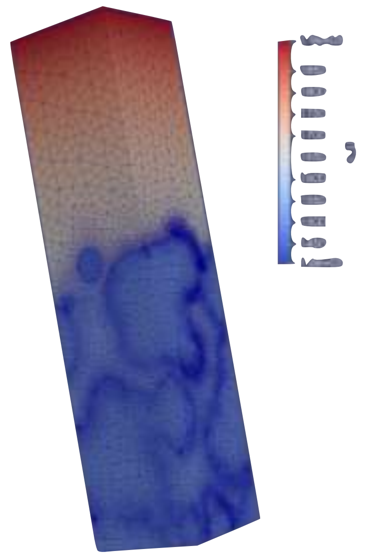
Virtual batteries

multi-scale, multi-physics,
and HPC for the next generation of
energy storage materials.

- Micro-structural realism shall be captured
- Scientific disciplines must cross link
- Replace learning from mistakes by predictive science.

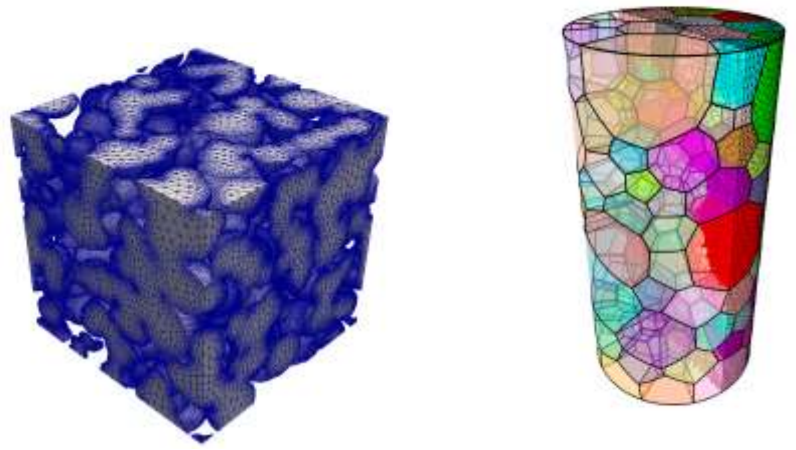
Mechanobiology





Energy storage

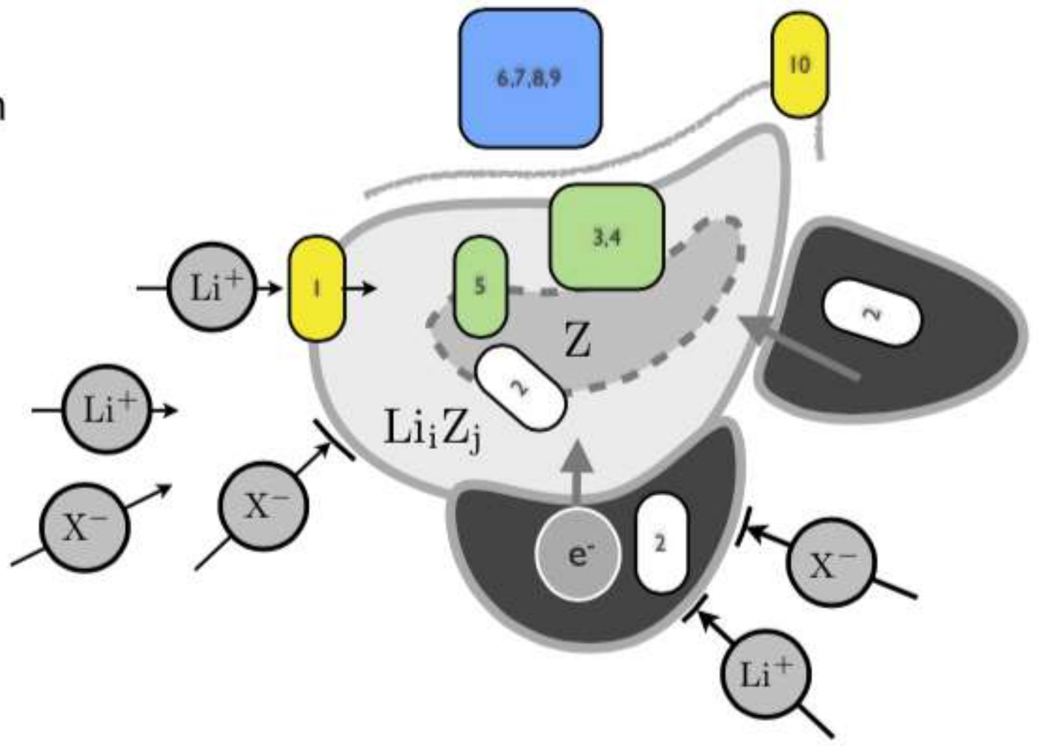
Multi scale characterization of materials



Processes and models

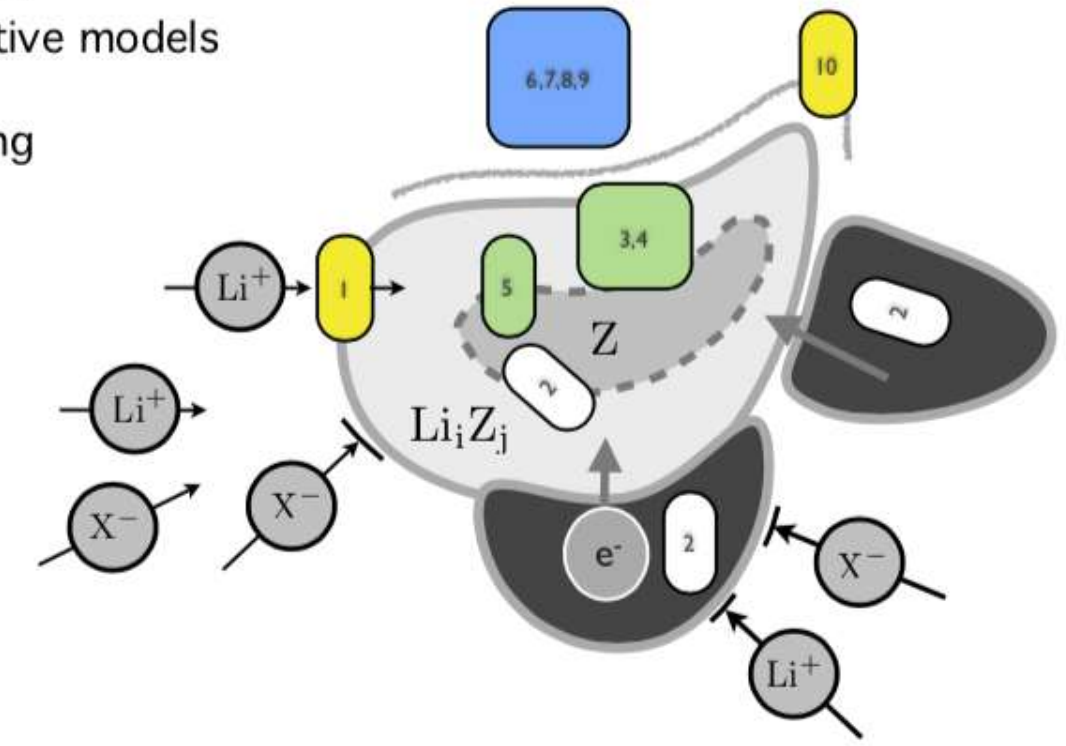
Processes

- 1 Intercalation reactions
- 2 Electronic conduction
- 3 Diffusion in active particles
- 4 Swelling, stress generation, failure
- 5 Phase segregation
- 6 Migration
- 7 Electrolysis
- 8 Ionic diffusion in the electrolyte
- 9 Ionization reaction / incomplete dissociation
- 10 SEI formation/disruption



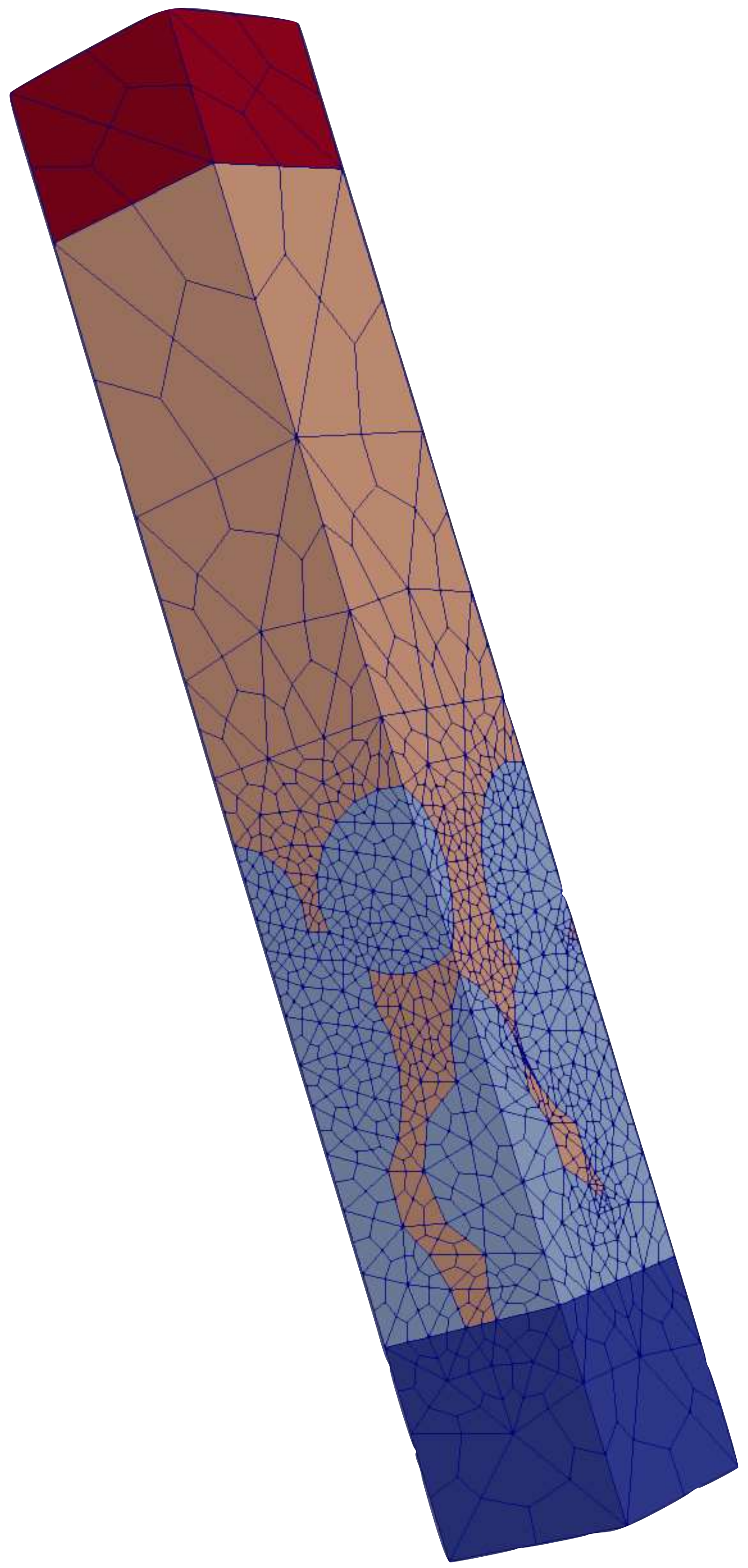
Models

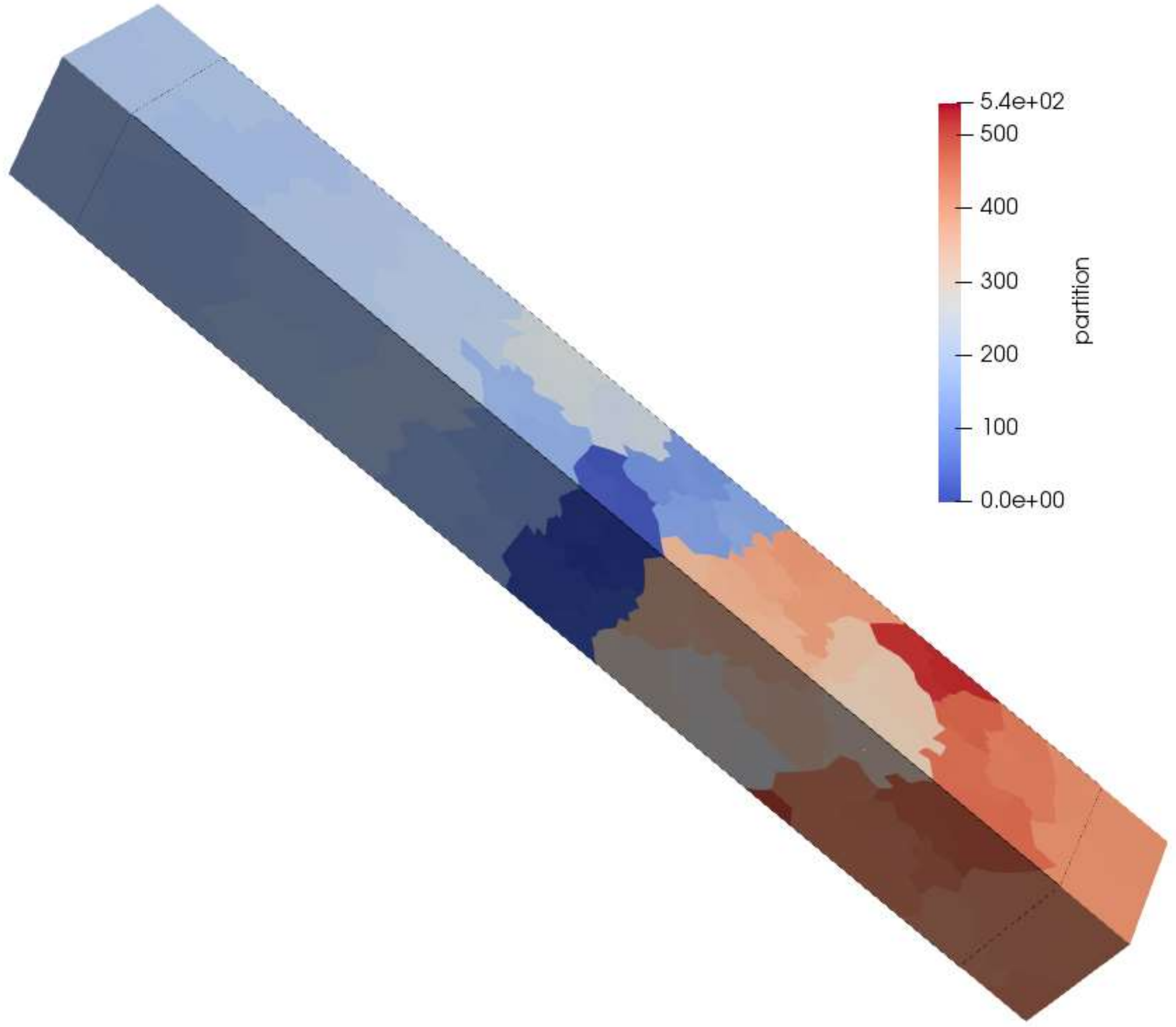
- 1 Butler-Volmer equation
Gouy-Chapman theory
- 2 Ohm's law
- 3 Mass balance equations
- 4 Principle of virtual power
TD consistent constitutive models
- 5 Sharp interface modeling
Cahn-Hilliard theory
- 6 Electroneutrality – Maxwell's equation in electro-quasi-statics
- 7 Faraday's law
- 8 Mass balance equations
- 9 Reaction rate in mass balance equations
- 10 SEI formation/disruption models



FEM implementation

deal.ii FEM HPC implementation





Discretization

381,036 cells
1,284,033 DOFs

Cores partition

8 nodes
544 cores
Marconi @ CINECA

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- Multiscale in electrodes
- Optimization of electrodes shape
- **Lithiated binders in thick cathodes**

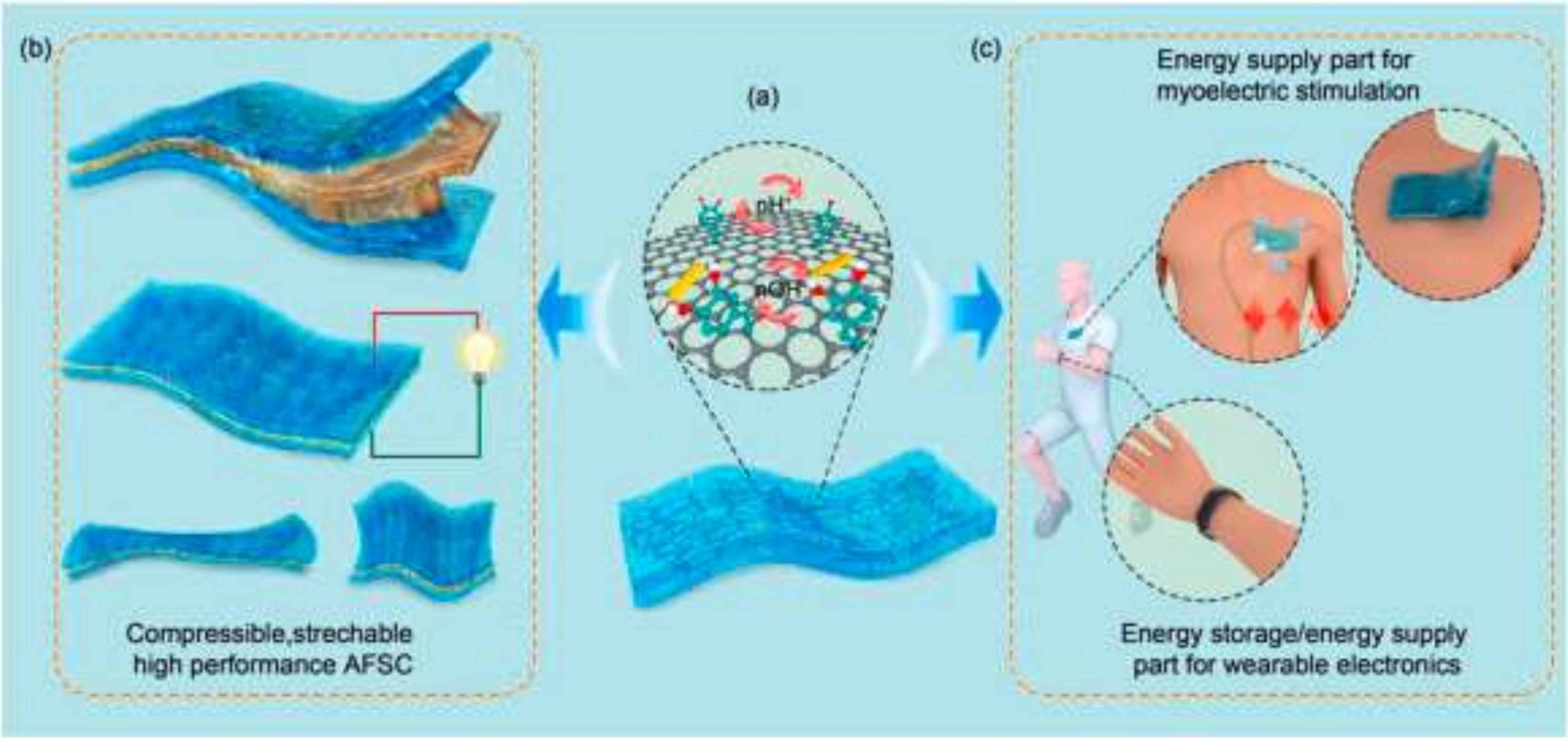
- Solid electrolytes conduction modeling
- Solid electrolytes dendritic growth
- Solid electrolytes deposition and stress evolution

- Gel polymer electrolytes

- Sodium batteries

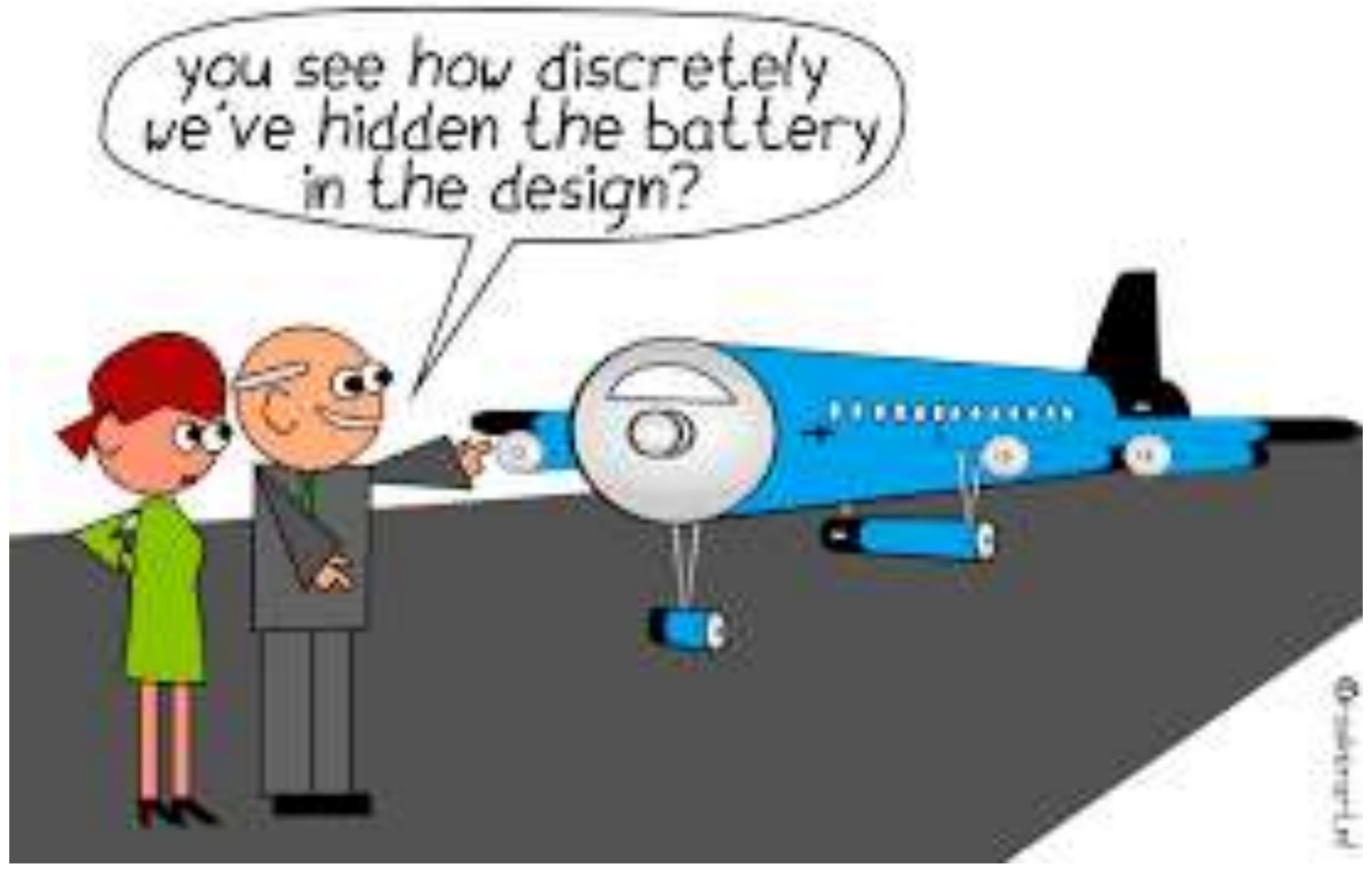
Gel polymer electrolytes systems

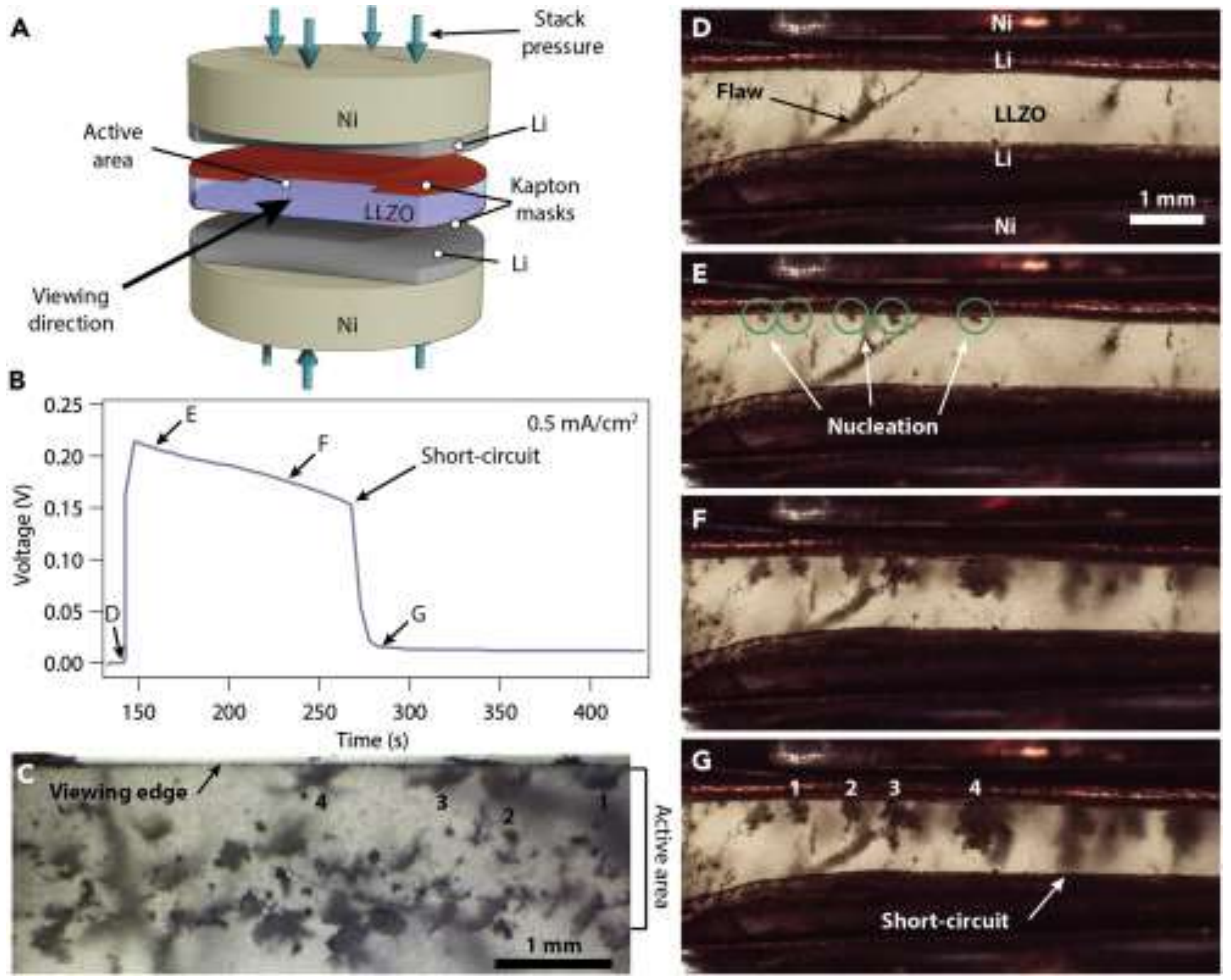
The increasing popularity of portable/wearable multifunctional electronic devices has highlighted the need for multifunctional power-supply devices such as self-adhesive, compressive, flexible, and stretchable all- hydrogel-based multifunctional supercapacitors (AFSC).

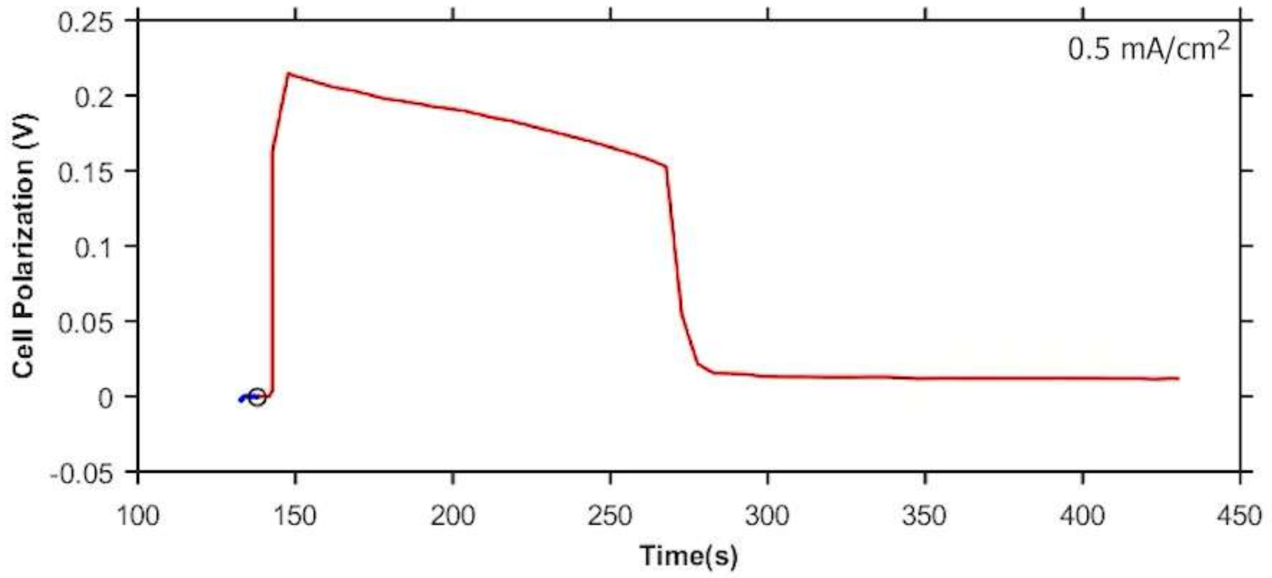


Lili Jiang, Youjian Li, Fa Zou, Donglin Gan, Mingyuan Gao, Le Yuan, Qinyong Zhang, Xiong Lu,
Highly self-adhesive, compressible, stretchable, all hydrogel-based supercapacitor for wearable/portable electronics,
Materials Today Physics,
Volume 33,
2023,
101046,

Solid electrolytes dendritic growth







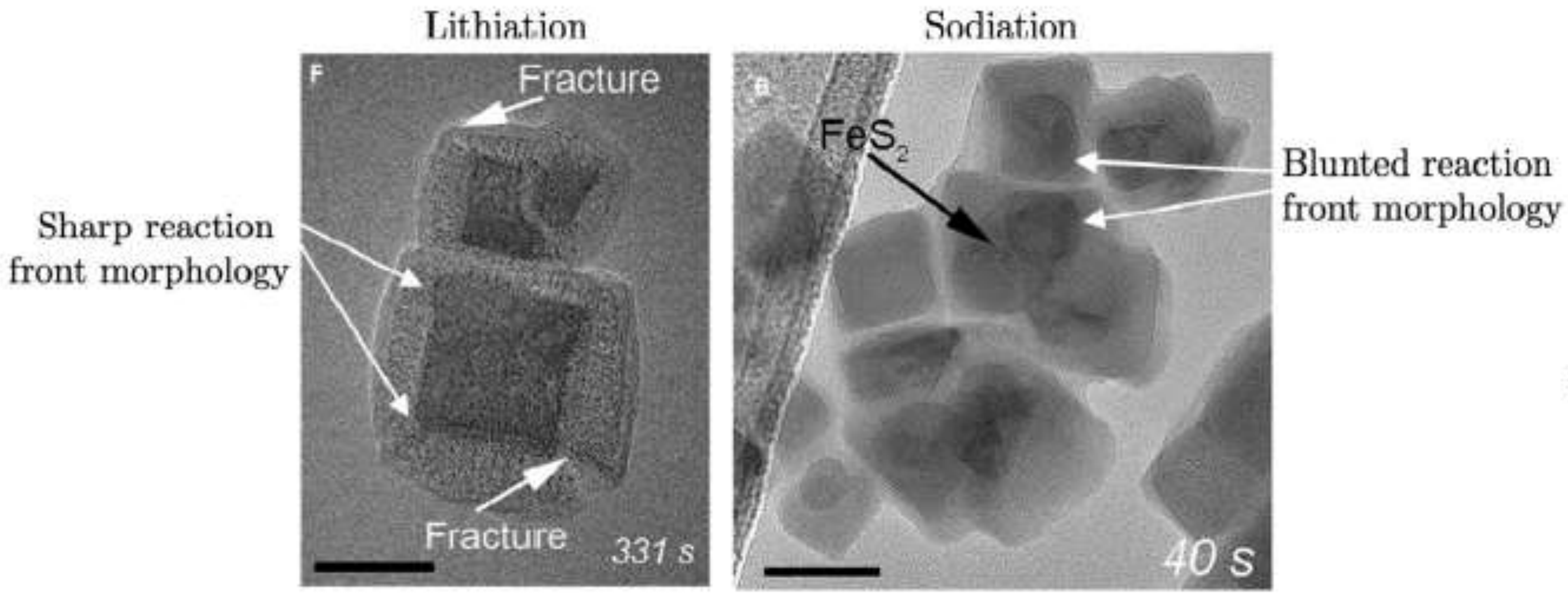
Eric Kazyak, Regina Garcia-Mendez, William S. LePage, Asma Sharafi, Andrew L. Davis, Adrian J. Sanchez, Kuan-Hung Chen, Catherine Haslam, Jeff Sakamoto, Neil P. Dasgupta, Li Penetration in Ceramic Solid Electrolytes: Operando Microscopy Analysis of Morphology, Propagation, and Reversibility, Matter, Volume 2, Issue 4, 2020, Pages 1025-1048, ISSN 2590-2385, https://doi.org/10.1016/j.matt.2020.02.008.

Sodium batteries

中科海钠
HiNa BATTERY

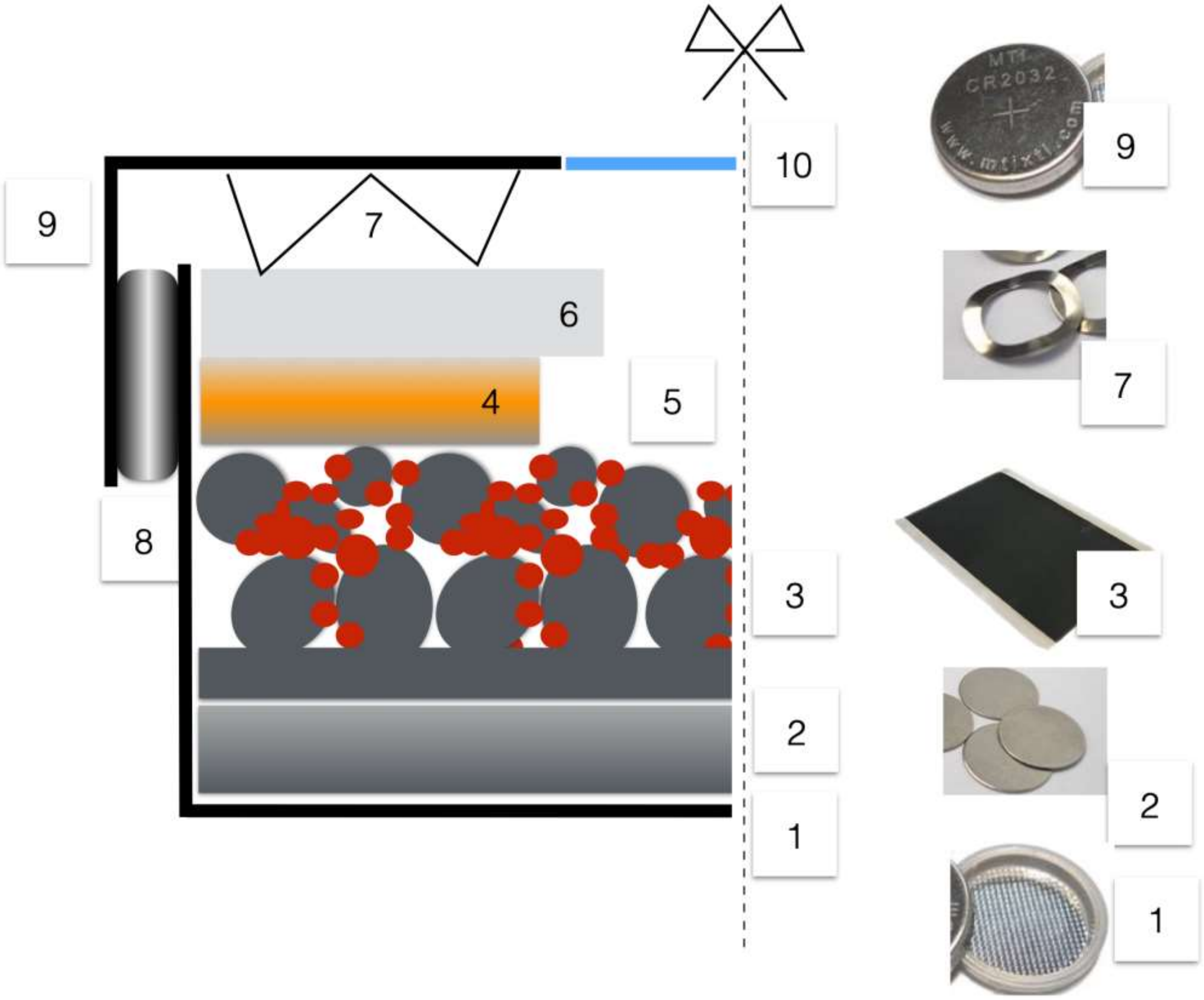
Hina Battery and Sehol, a joint venture between JAC and Volkswagen Anhui, have jointly built a sodium-ion battery test vehicle based on the Sehol EX10 small electric car.

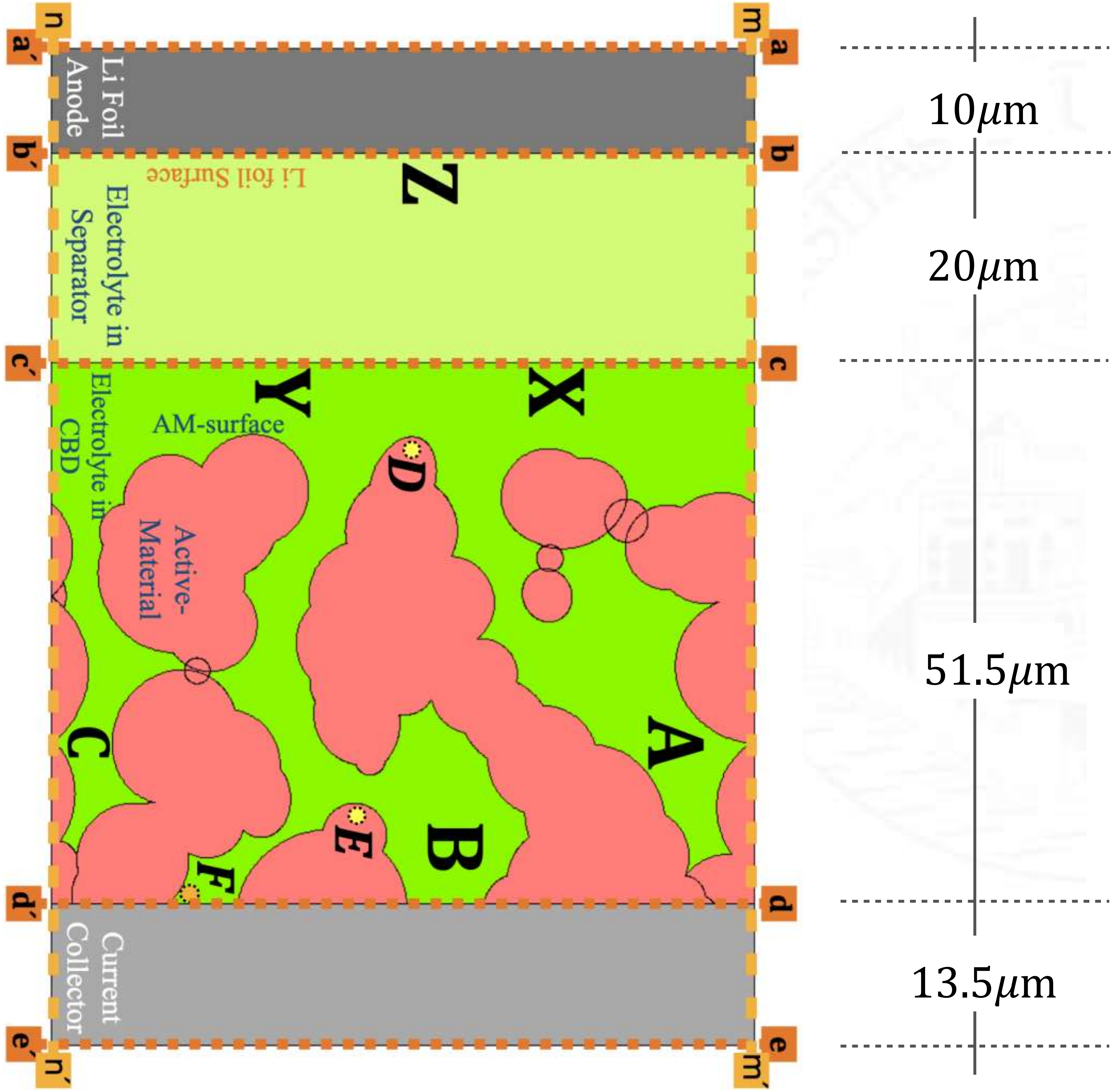
Sodium batteries



Analisi computazionale ad elementi finiti per materiali anodici a lega per batterie ioni sodio

Lithiated binders in thick cathodes





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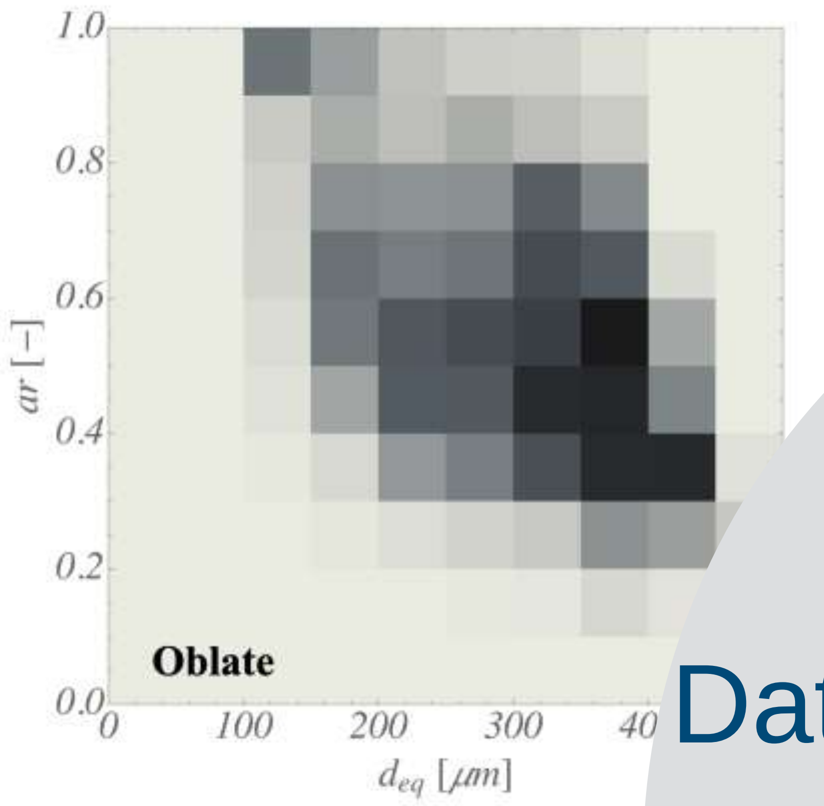
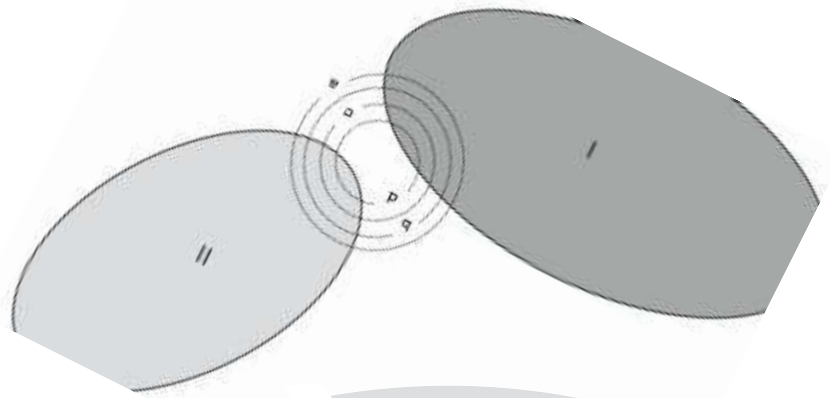
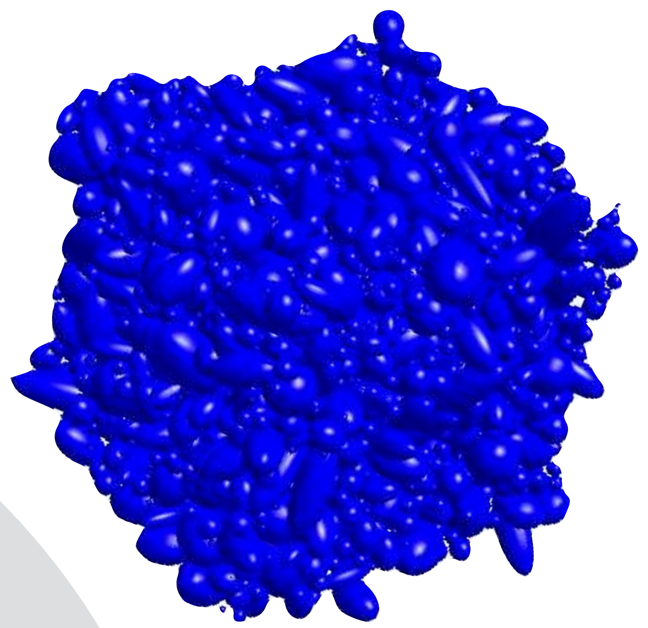
Lithiated binders in thick cathodes

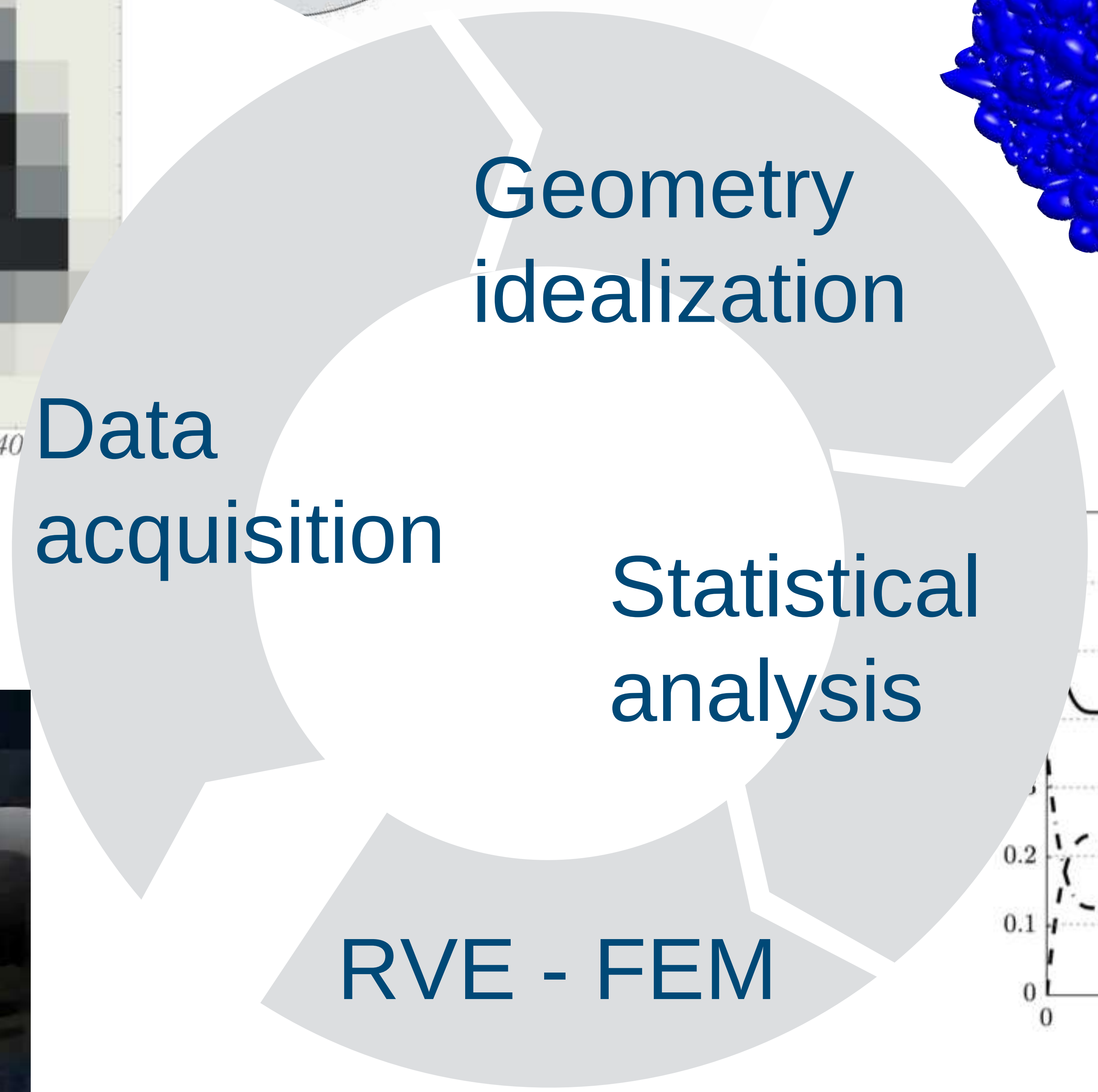
Pdf of experimental data in terms of selected morphological metrics



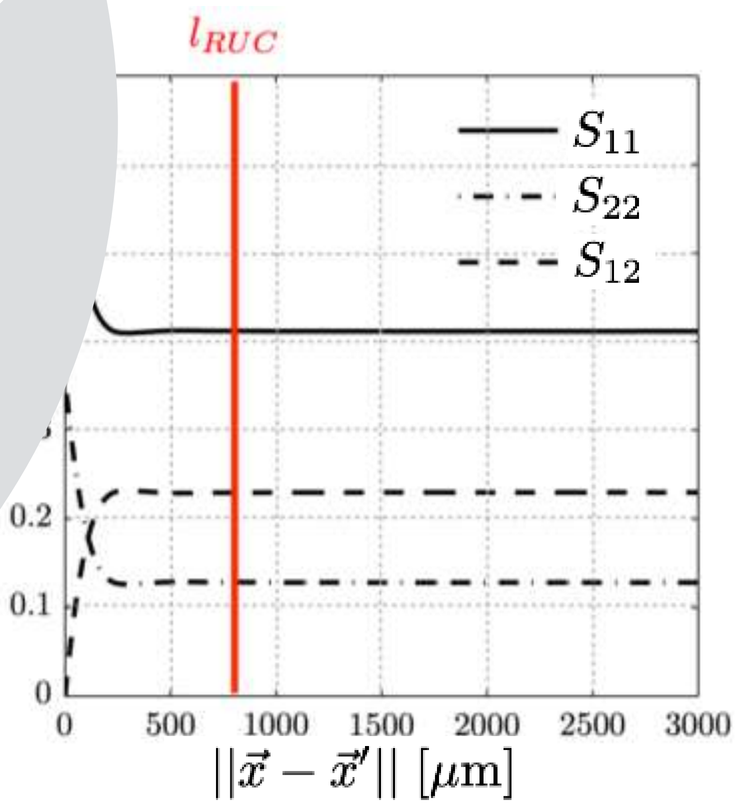




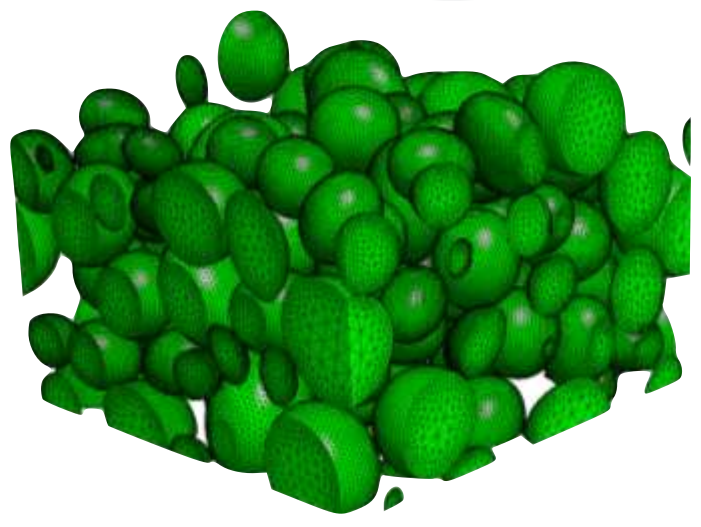
Percolated pack from data, obtained using sophisticated computational geometry algorithms



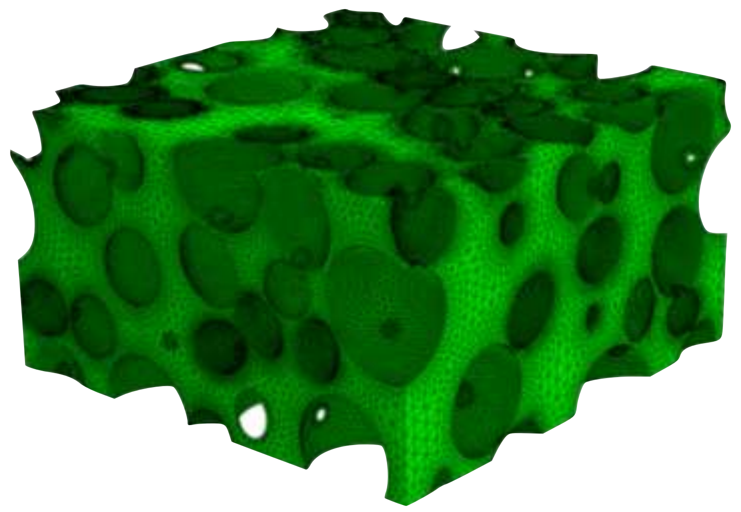
The characteristic size of the RUC is estimated via second order statistical descriptors



An example of particle acquisition via flowcam



LiCoO2



carbon and polymeric binder

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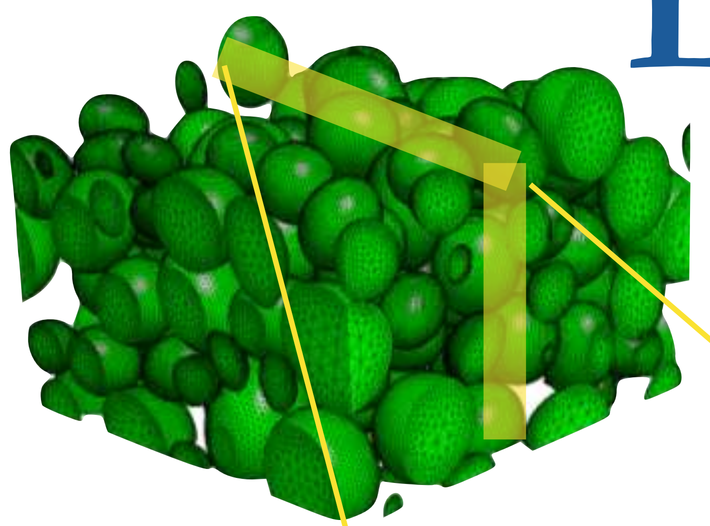
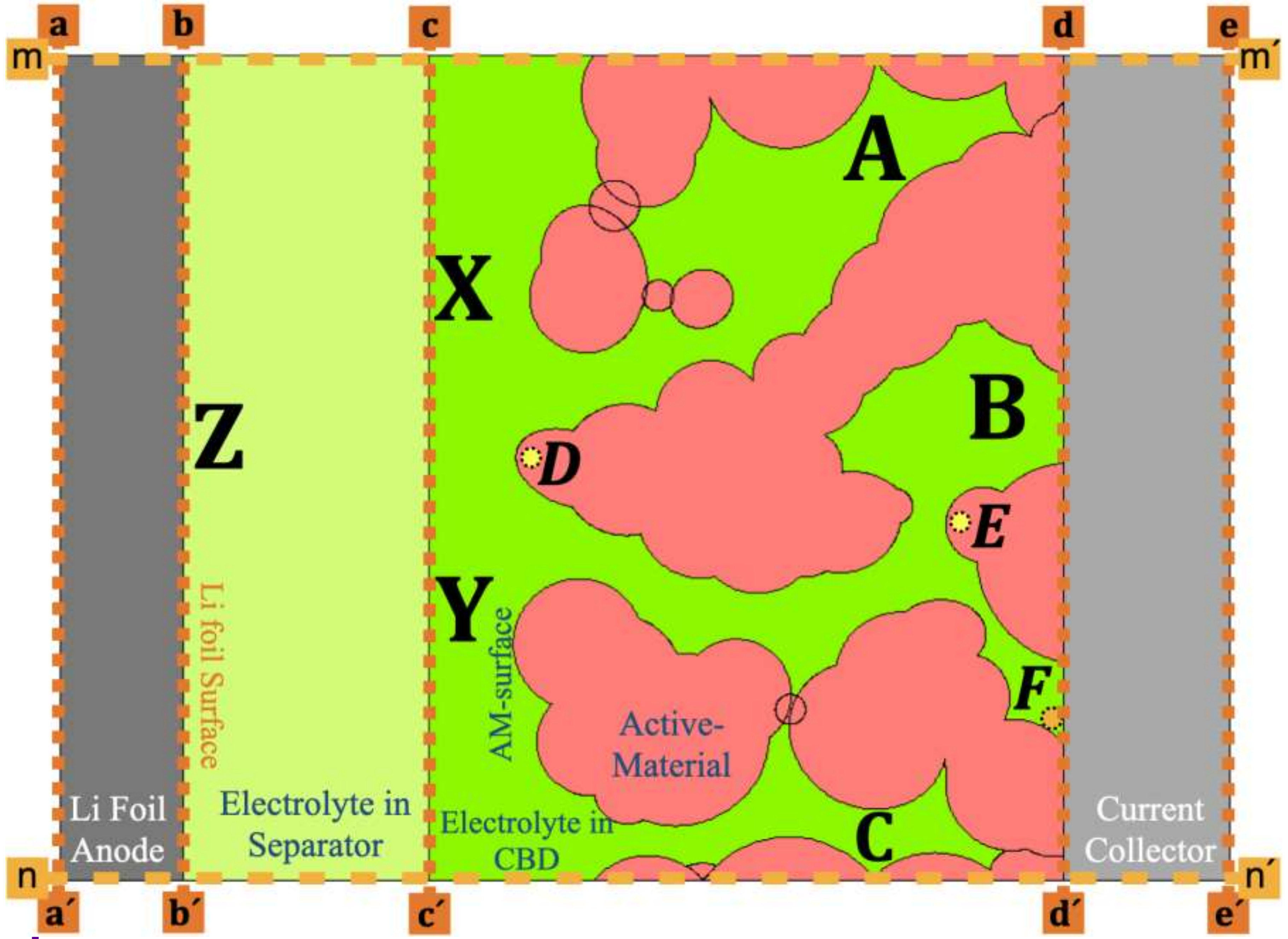
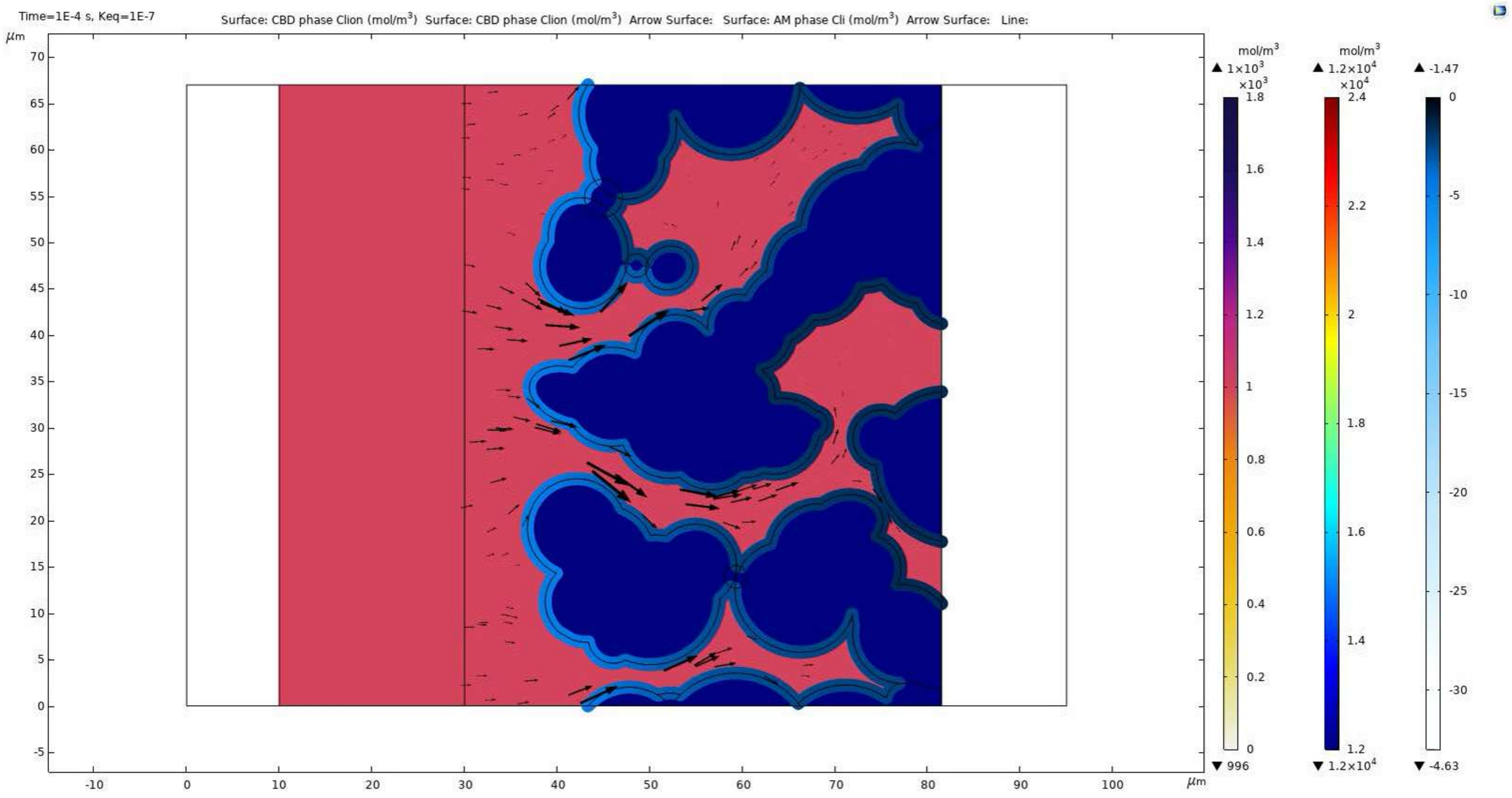
Lithiated binders in thick cathodes

Inactive binder half-cell discharged at 1C-rate







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Lithiated binders in thick cathodes

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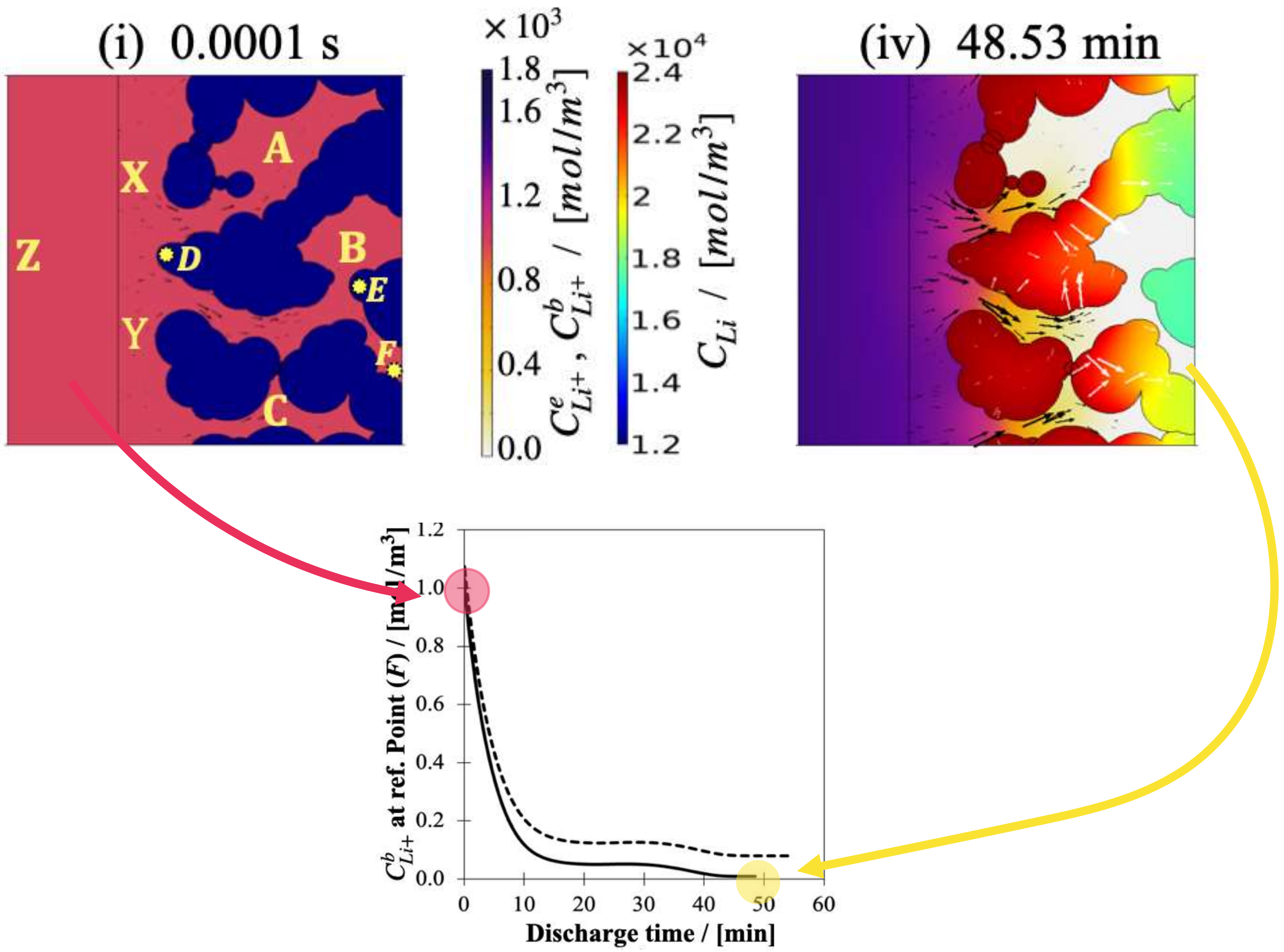
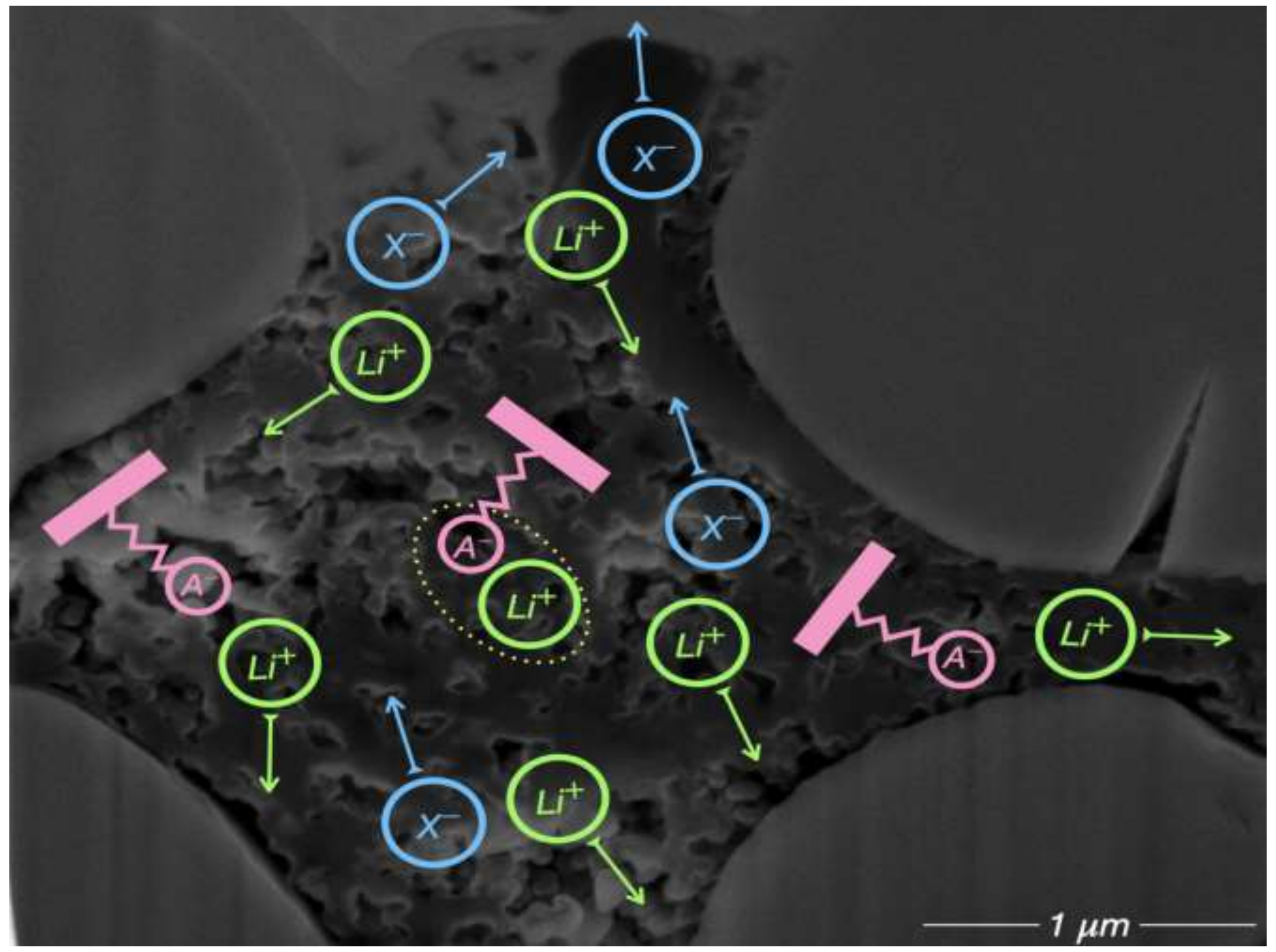


Active polymer binders



Active polymer binders

Blending either lithium sulfonate functionalized nanoparticles (SFNPLi) or lithiated ion conducting polymer (Poly(STFSI)Li), with usual binder (PVDF).

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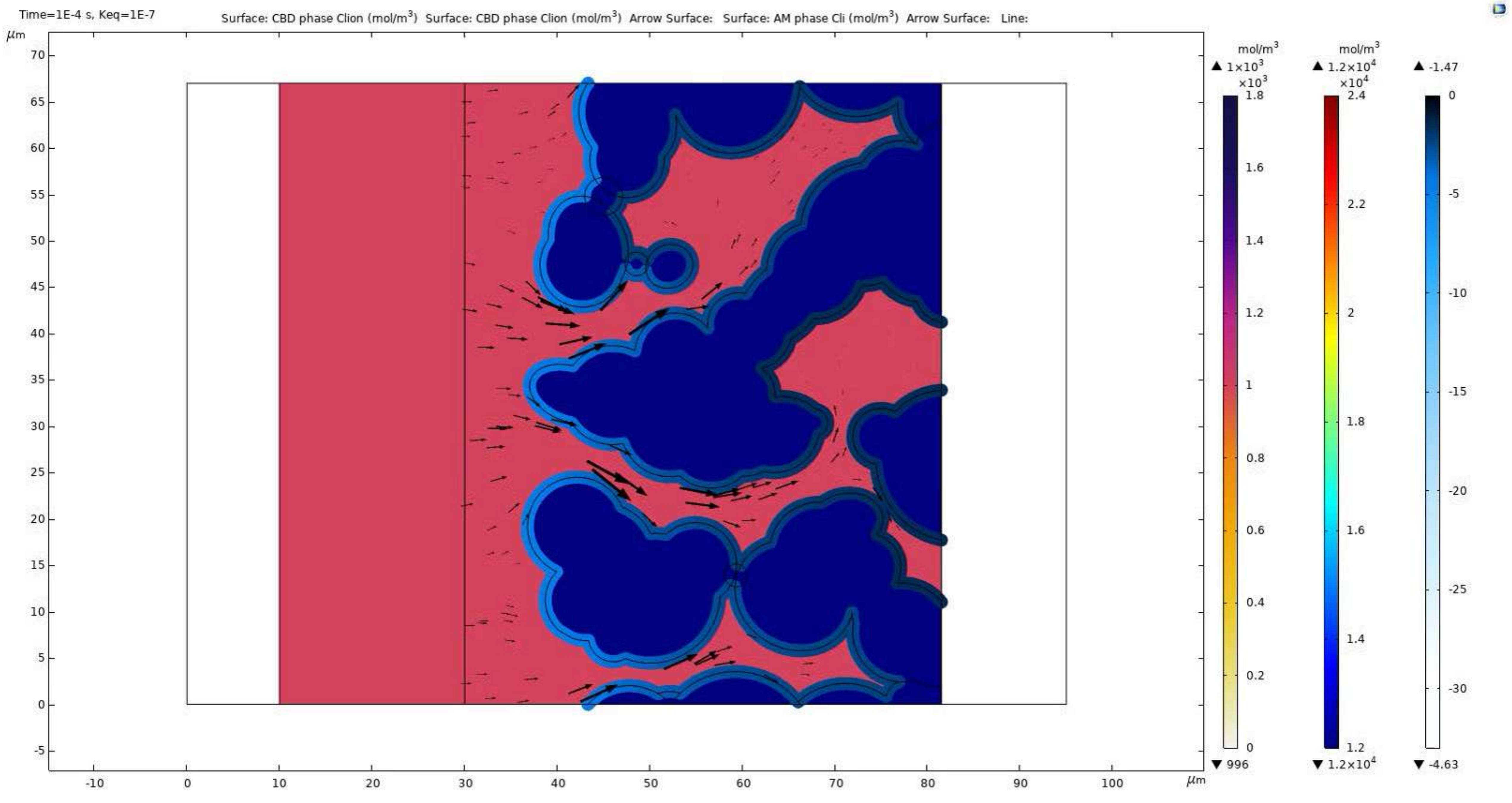
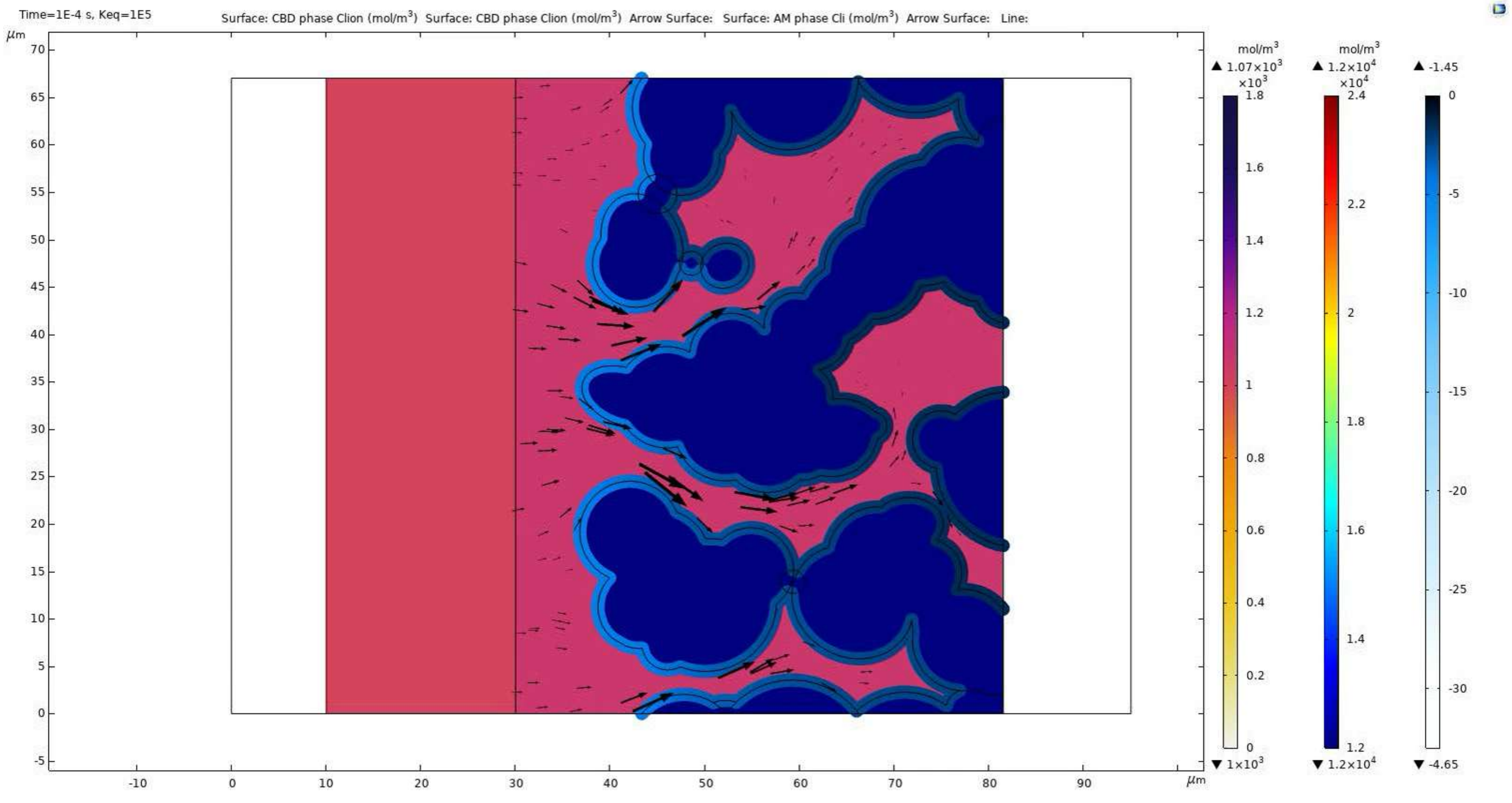
Cell simulations

Inactive vs active binder half-cell discharged at 1C-rate

Inactive



Active



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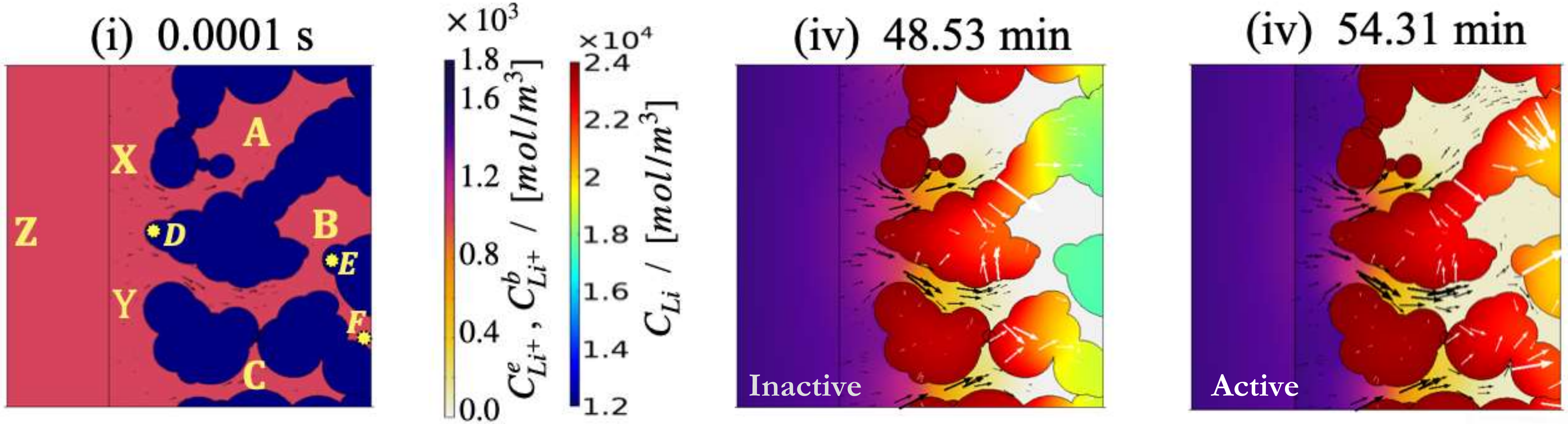
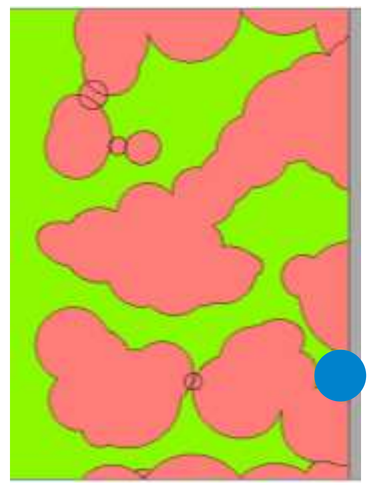
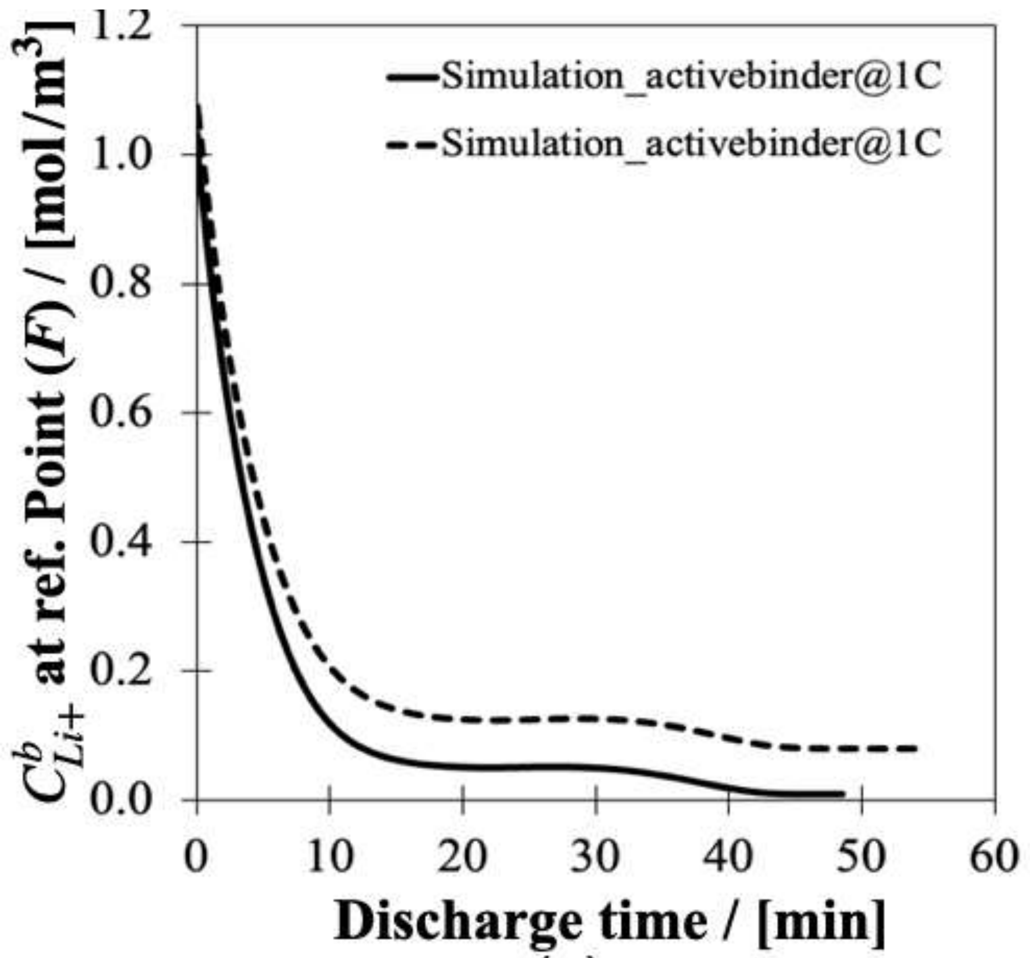
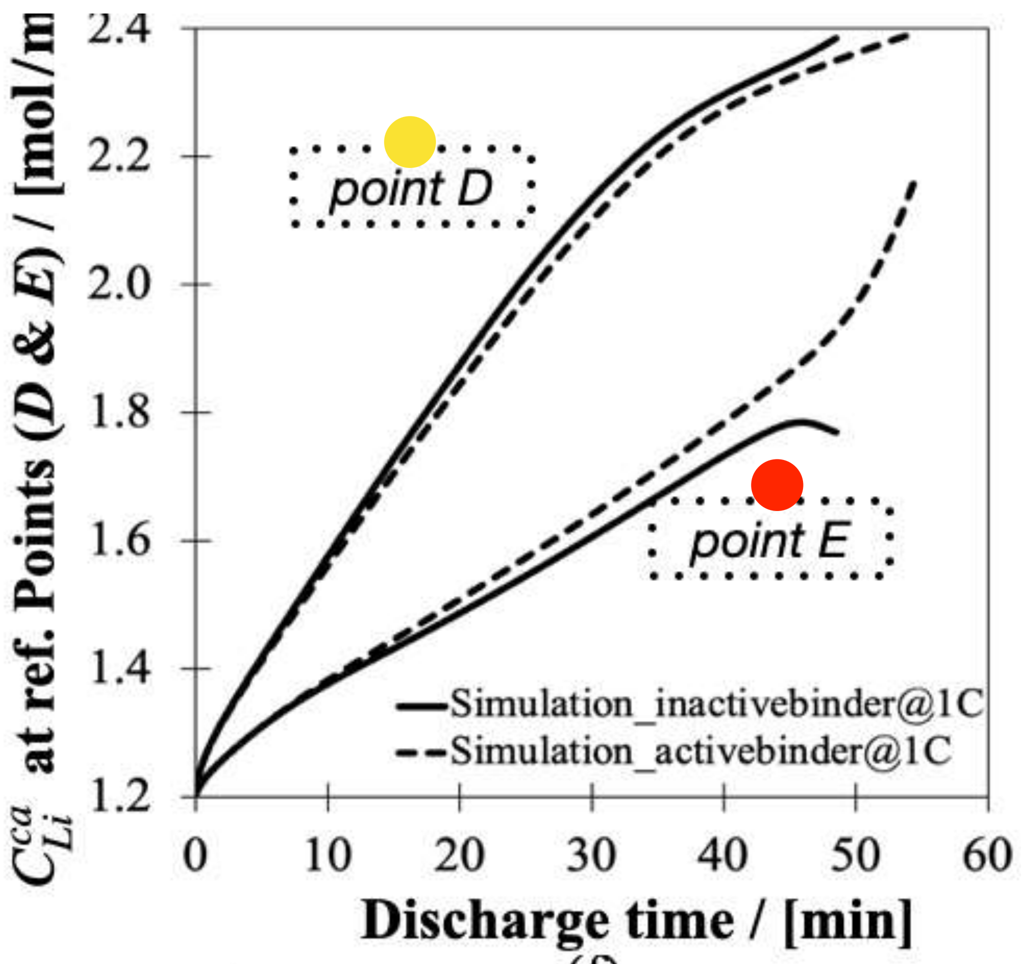


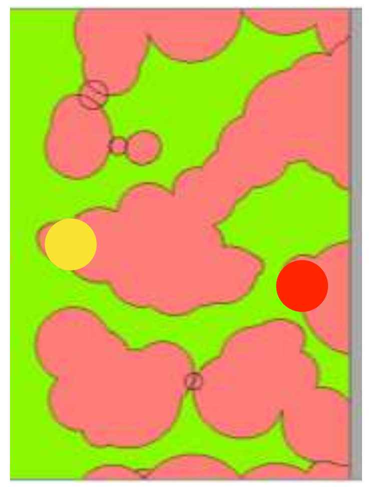




(e)



(f)



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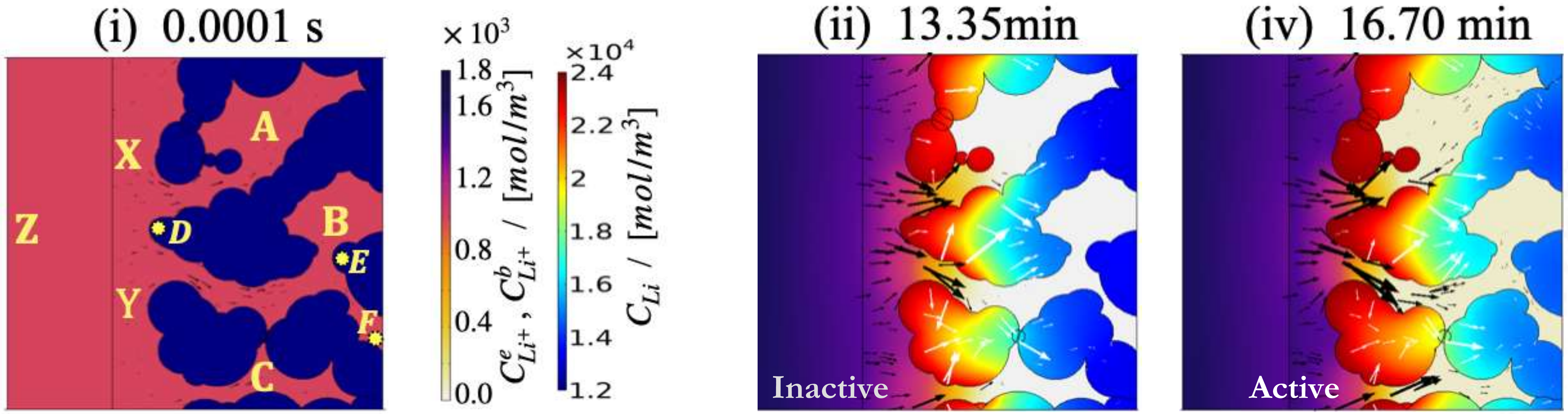
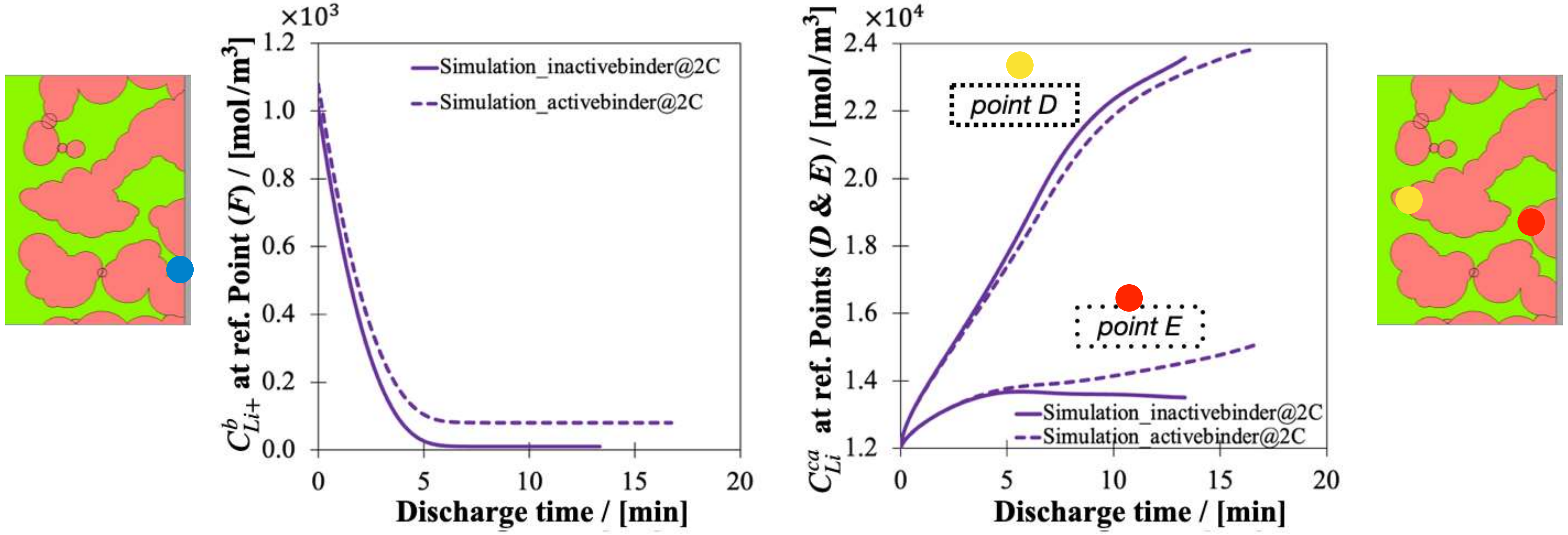
Cell simulations

Inactive vs active binder half-cell discharged at 2C-rate





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Shape optimization for electrodes

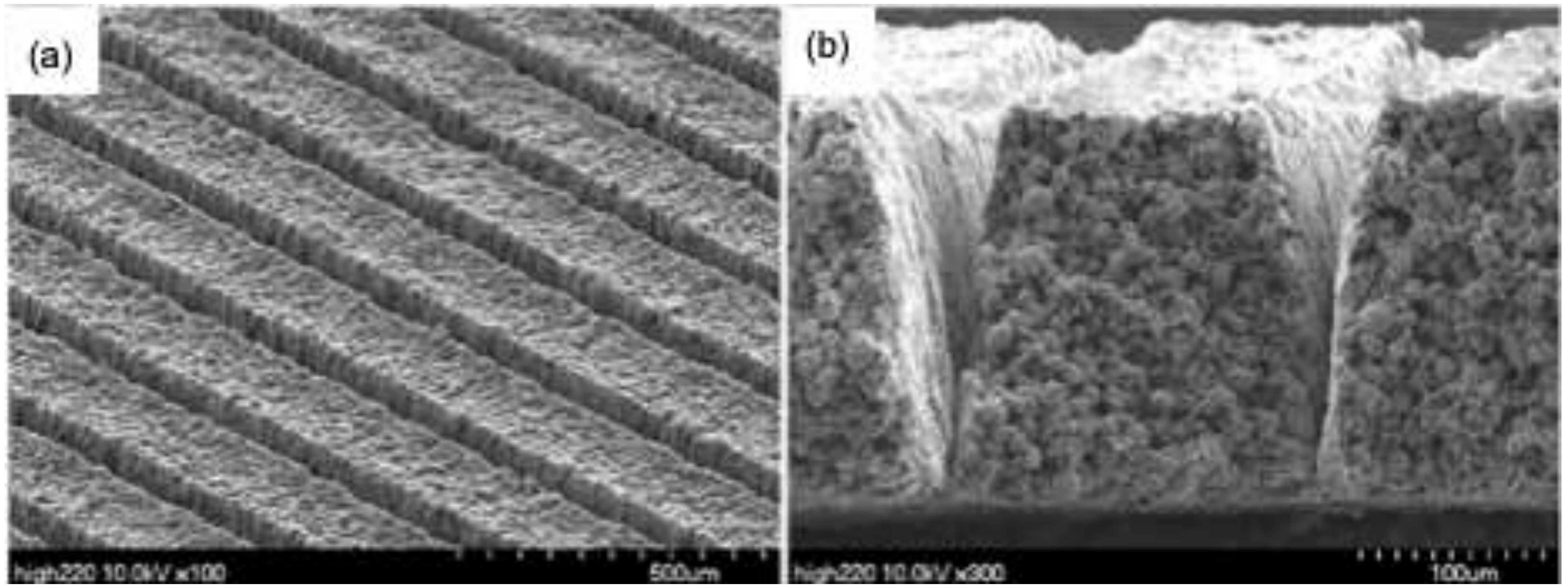
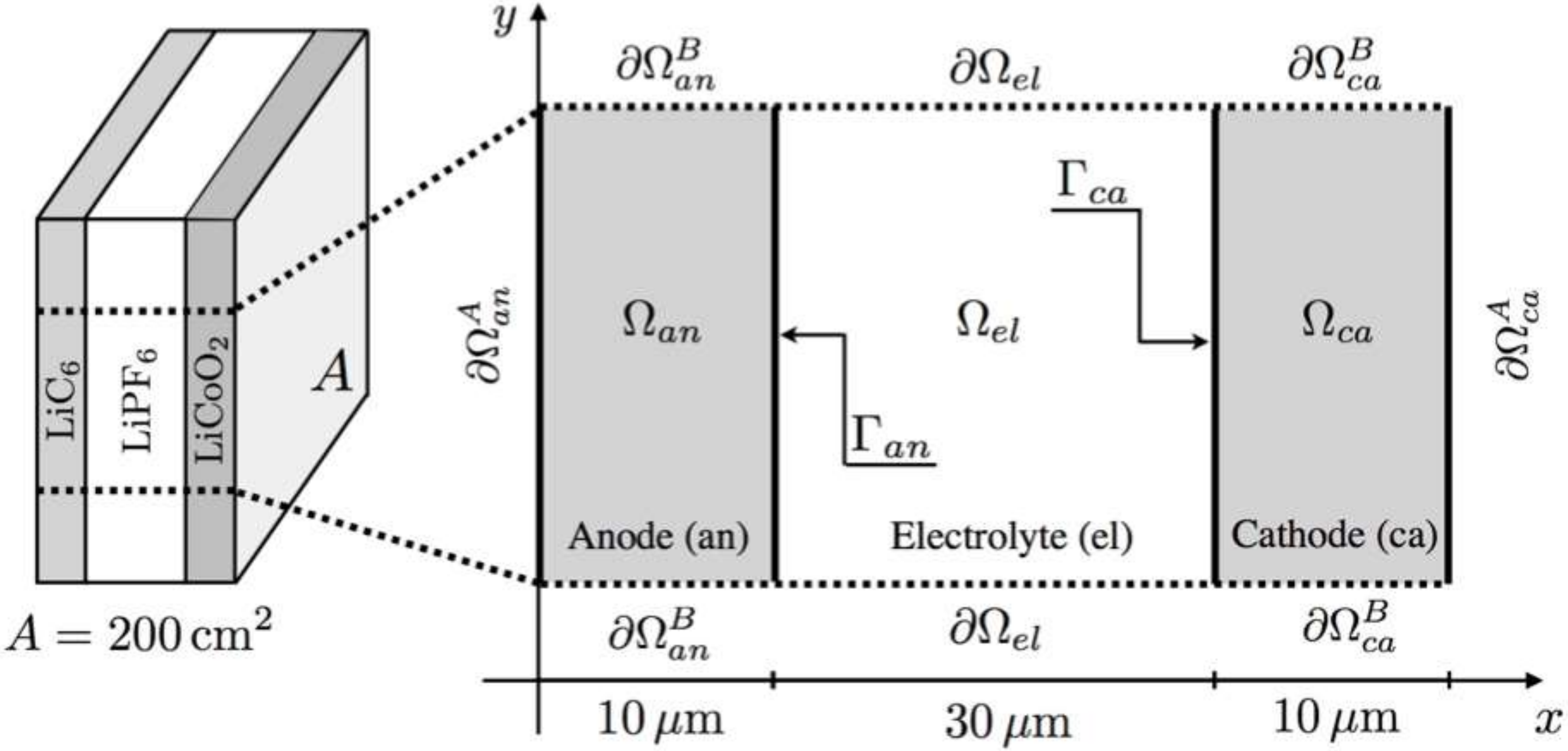


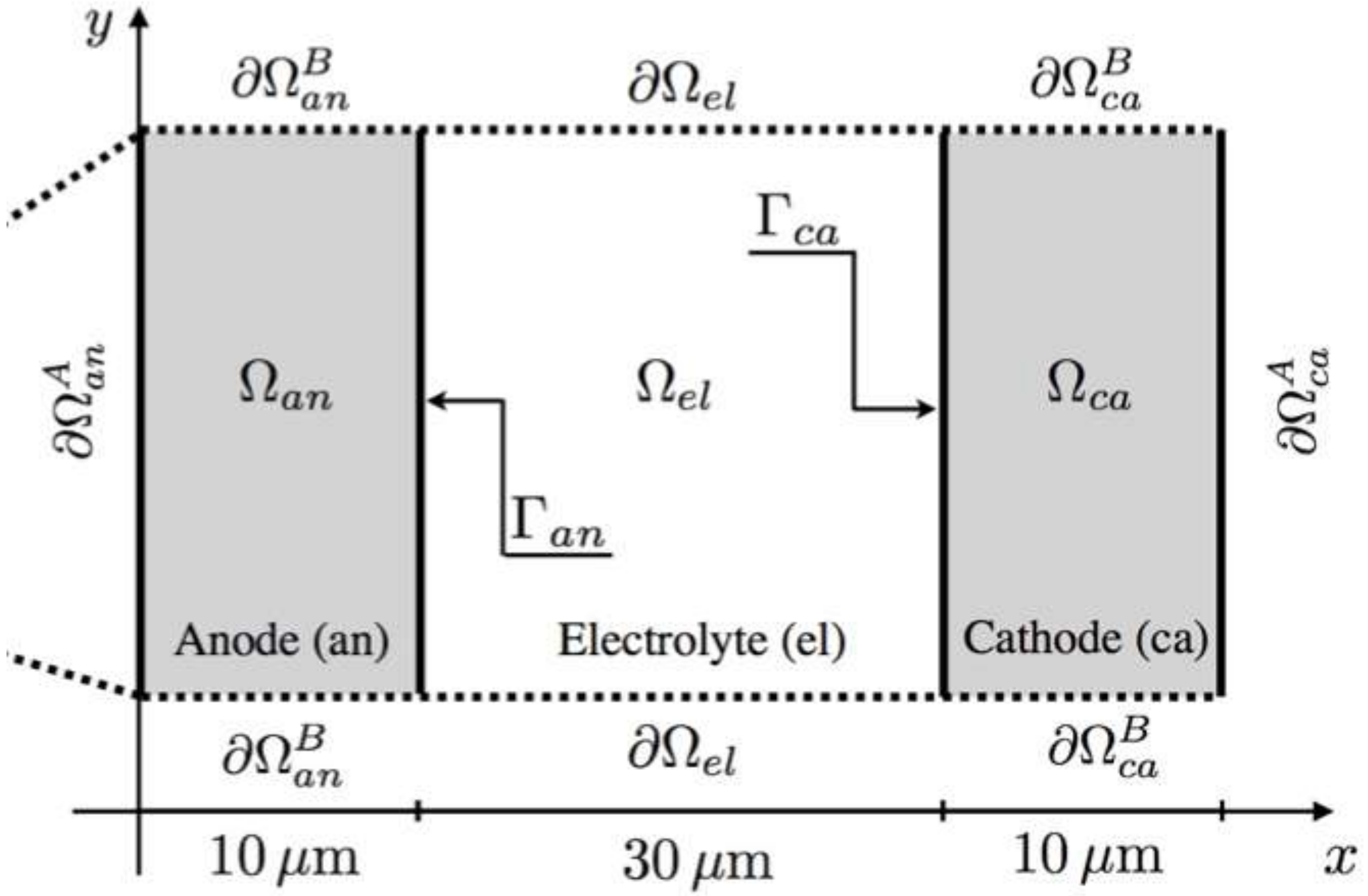
Figure 2: *SEM images of structured electrode a) structured electrode with high porosity. b) the cross section of structured electrode. Reprinted and adapted with permission from*

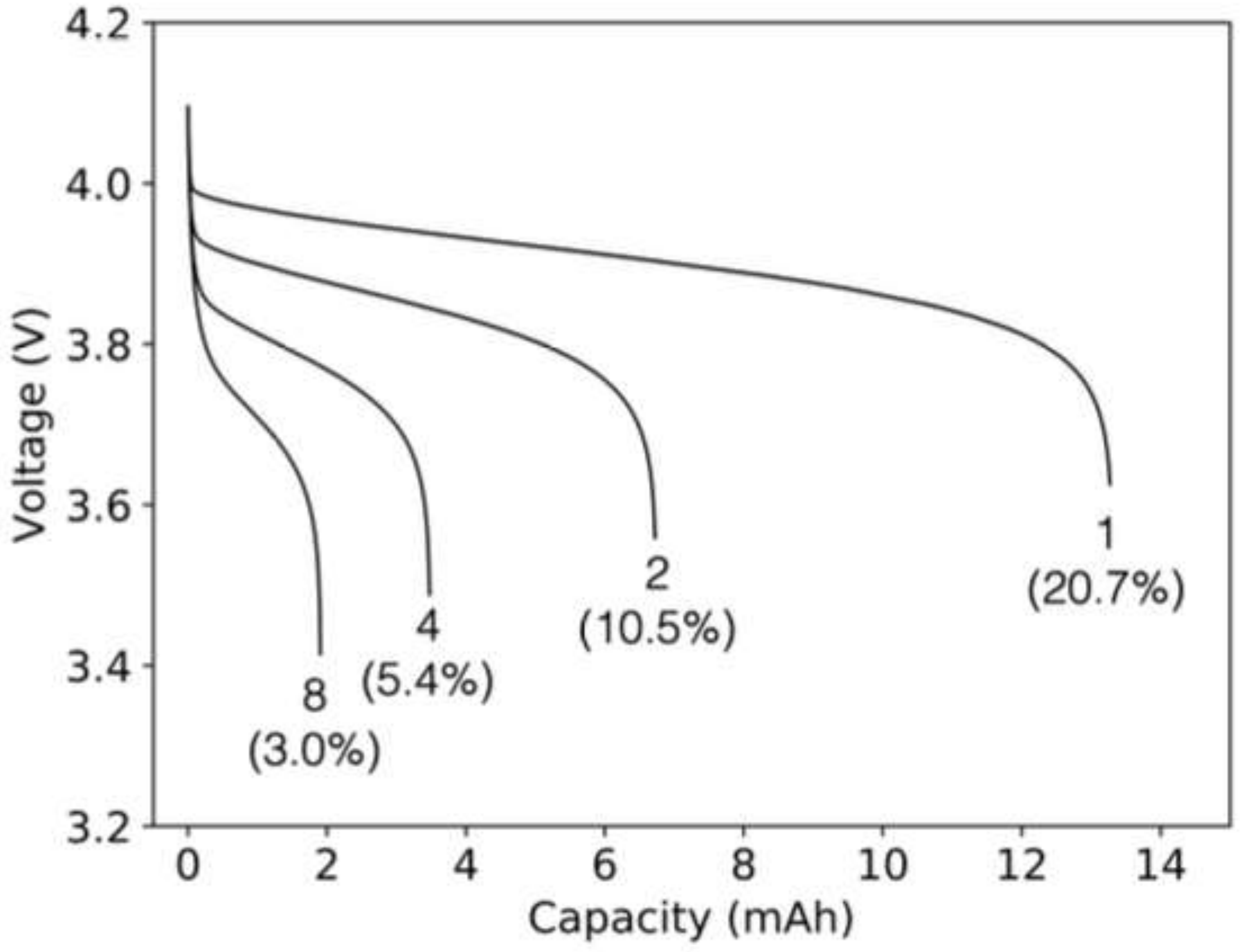
J. Park, S. Hyeon, S. Jeong, and H.-J. Kim. Performance enhancement of li-ion battery by laser structuring of thick electrode with low porosity. *J IND ENG CHEM*, 70:178–185, 2019.

Shape optimization for electrodes



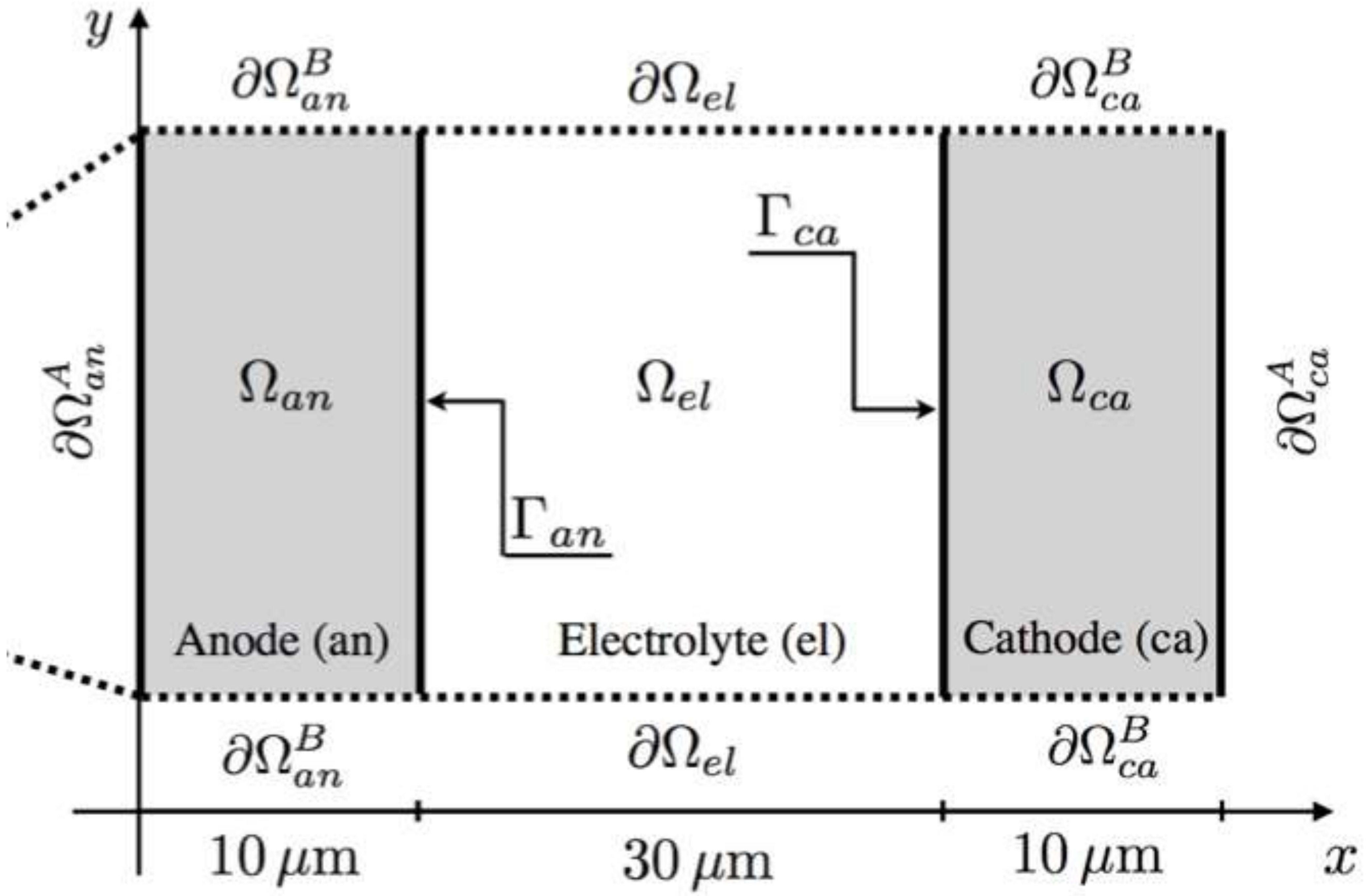
Shape optimization for electrodes



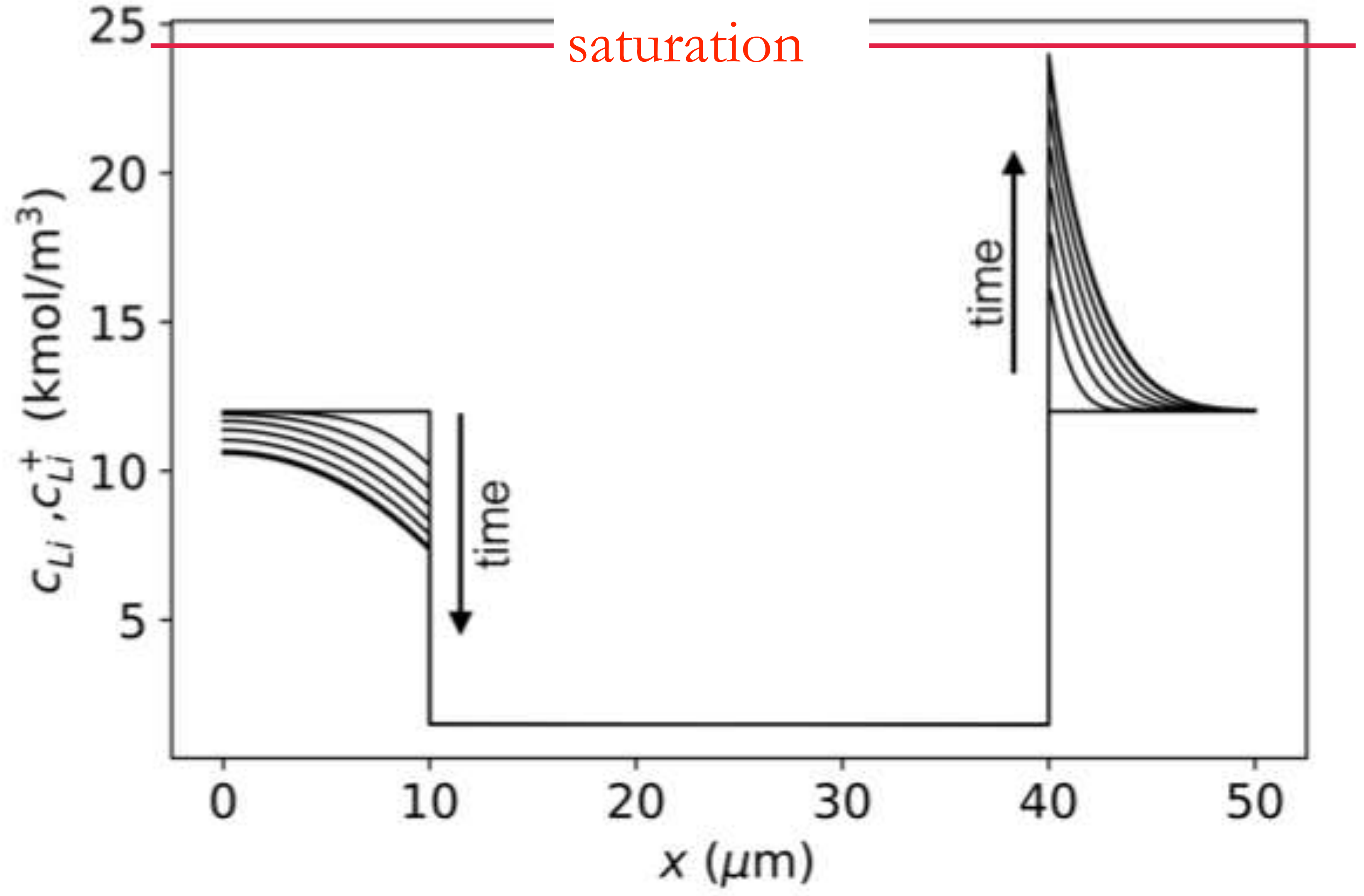


(b) Voltage vs capacity

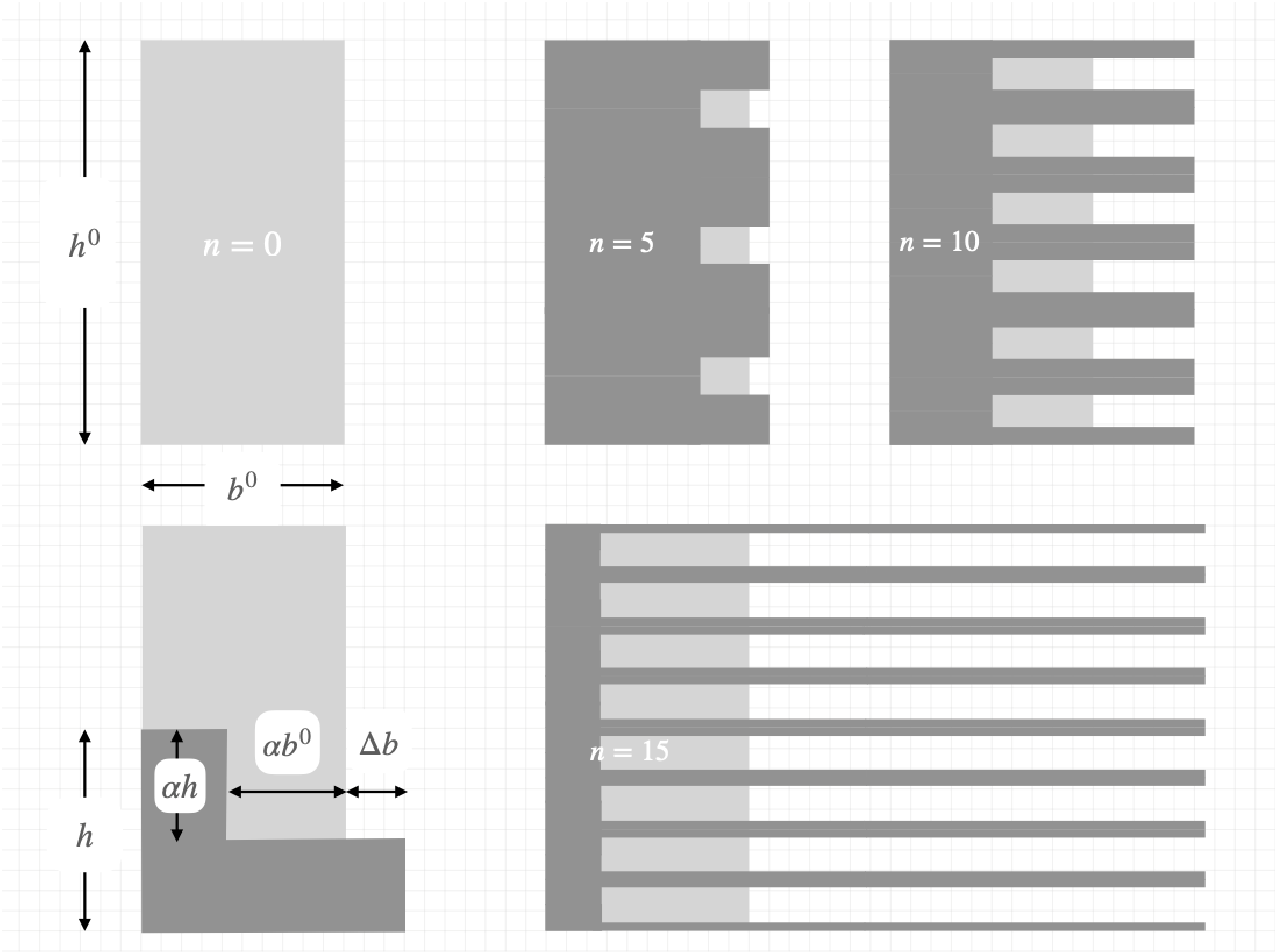
Shape optimization for electrodes



1C



Shape optimization for electrodes



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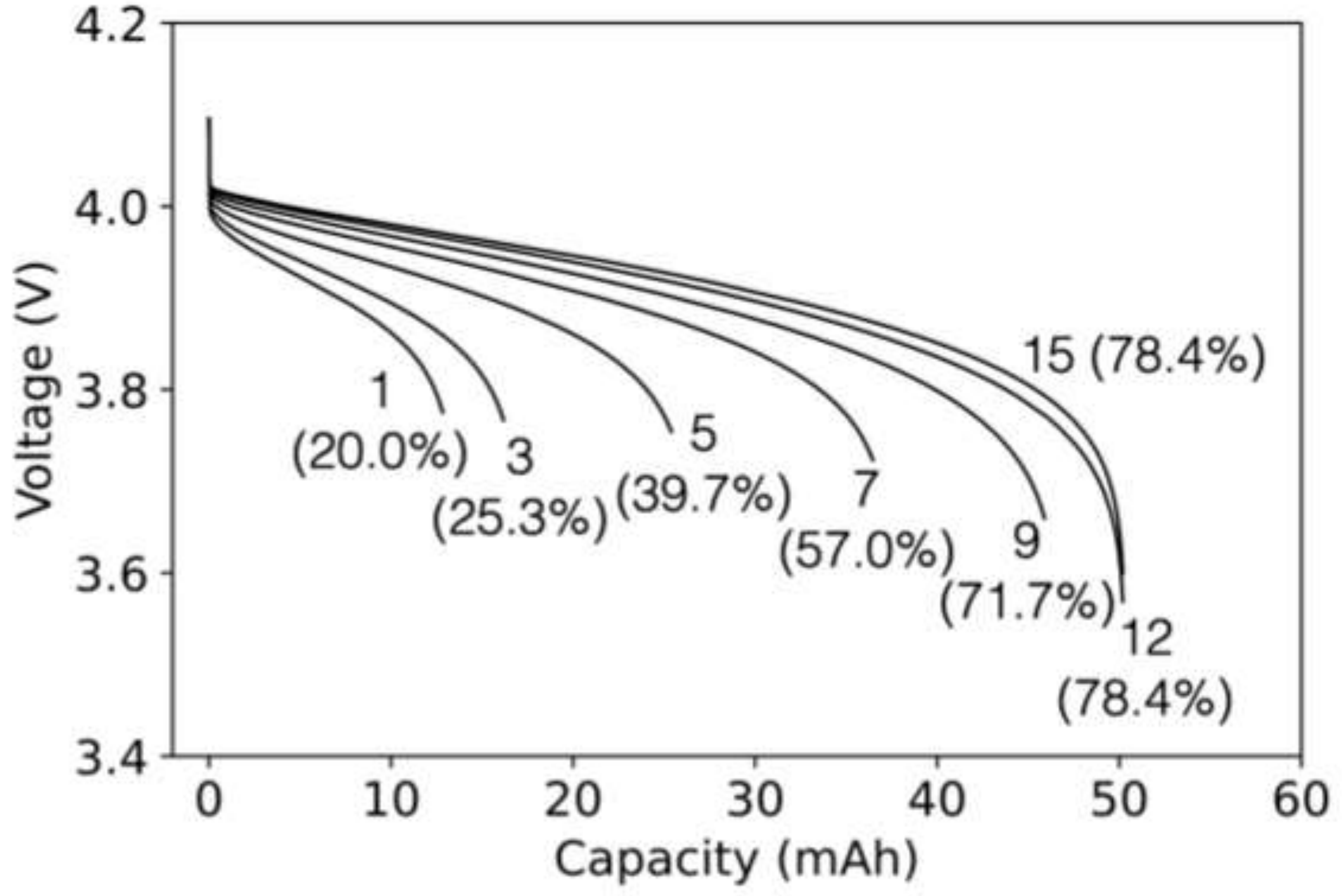
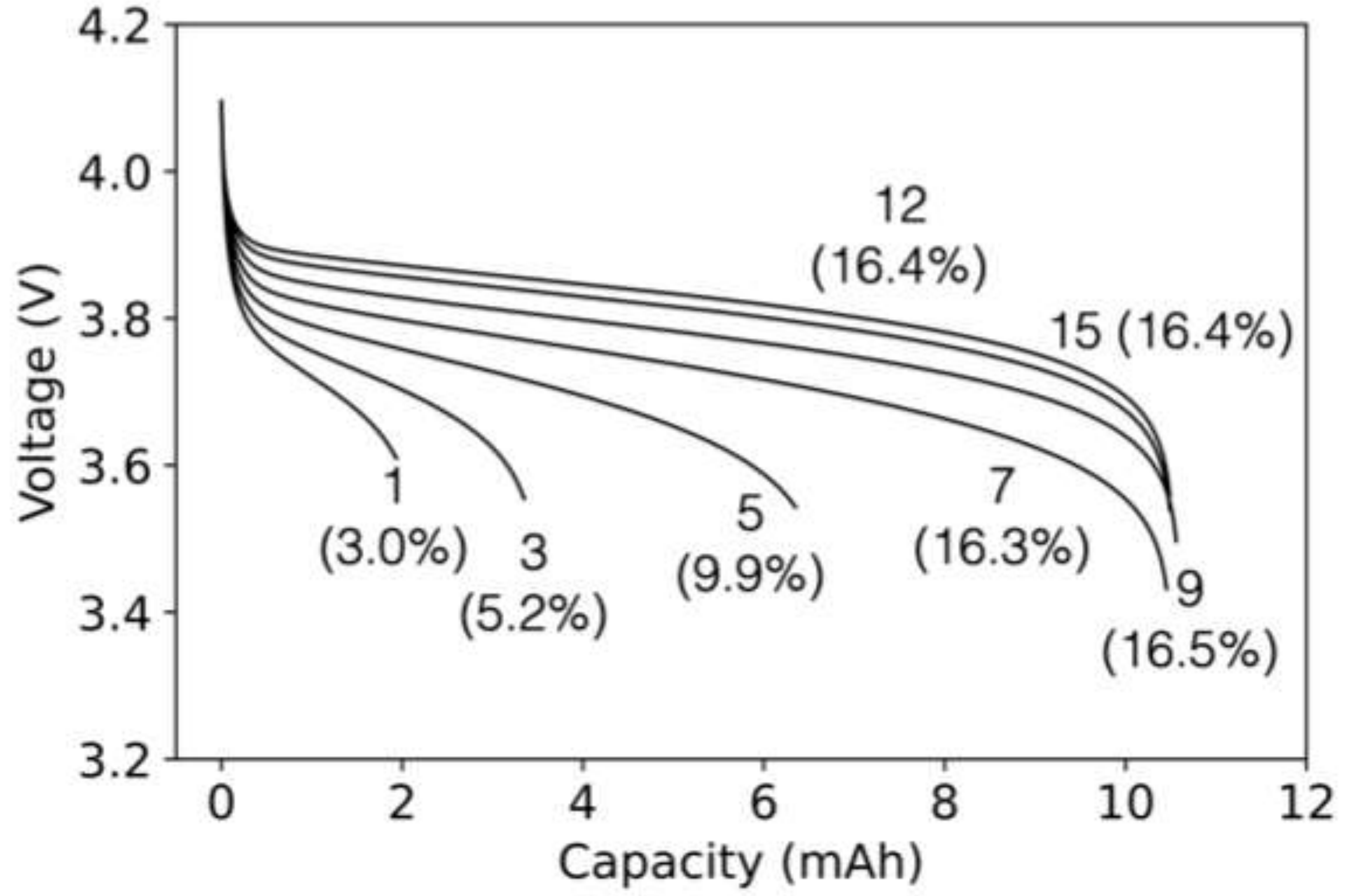
Shape optimization for electrodes



(a)



(b)

Figure 11: *Influence of cathode morphology on the simulated voltage for 1.0 (a) and 8.0 (b) C-rate discharging. Each voltage profile is labelled by the integer n, i.e. the constant that identifies the shape of cathode (see Fig. 4). The battery efficiency, reported in parenthesis, is computed as the ratio between the extracted charge at the end of the discharging and the theoretical capacity.*

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Shape optimization for electrodes

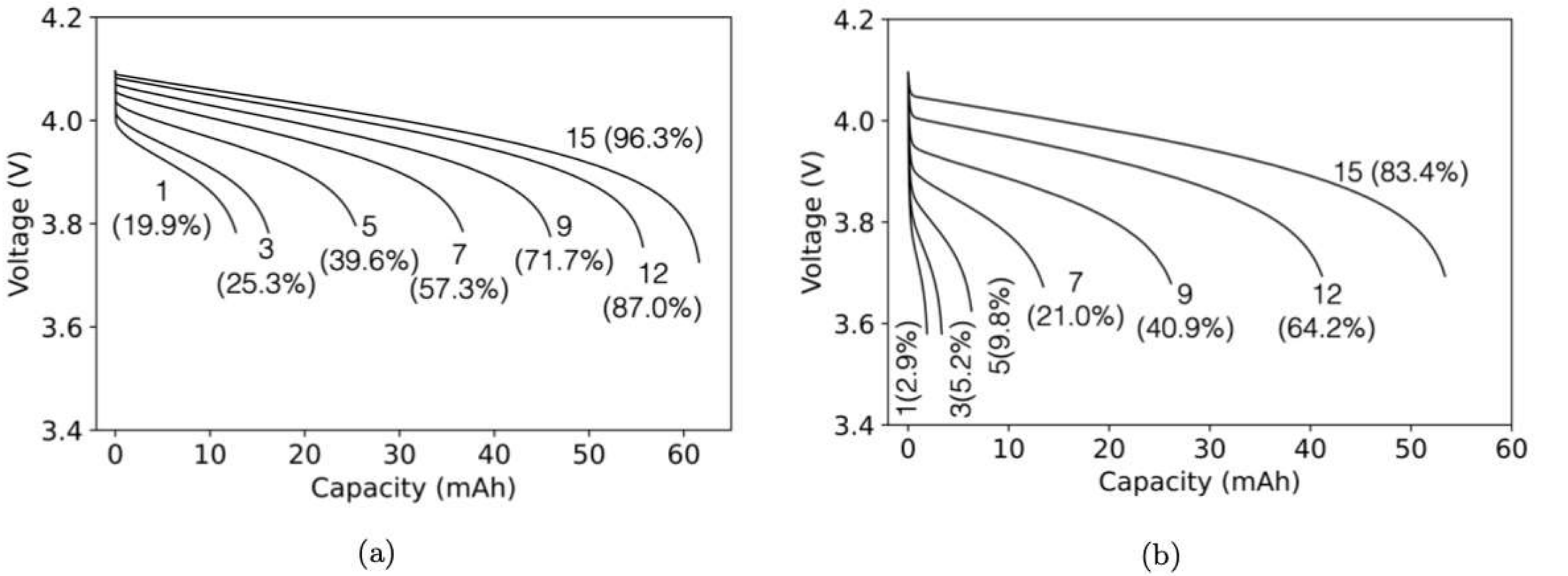
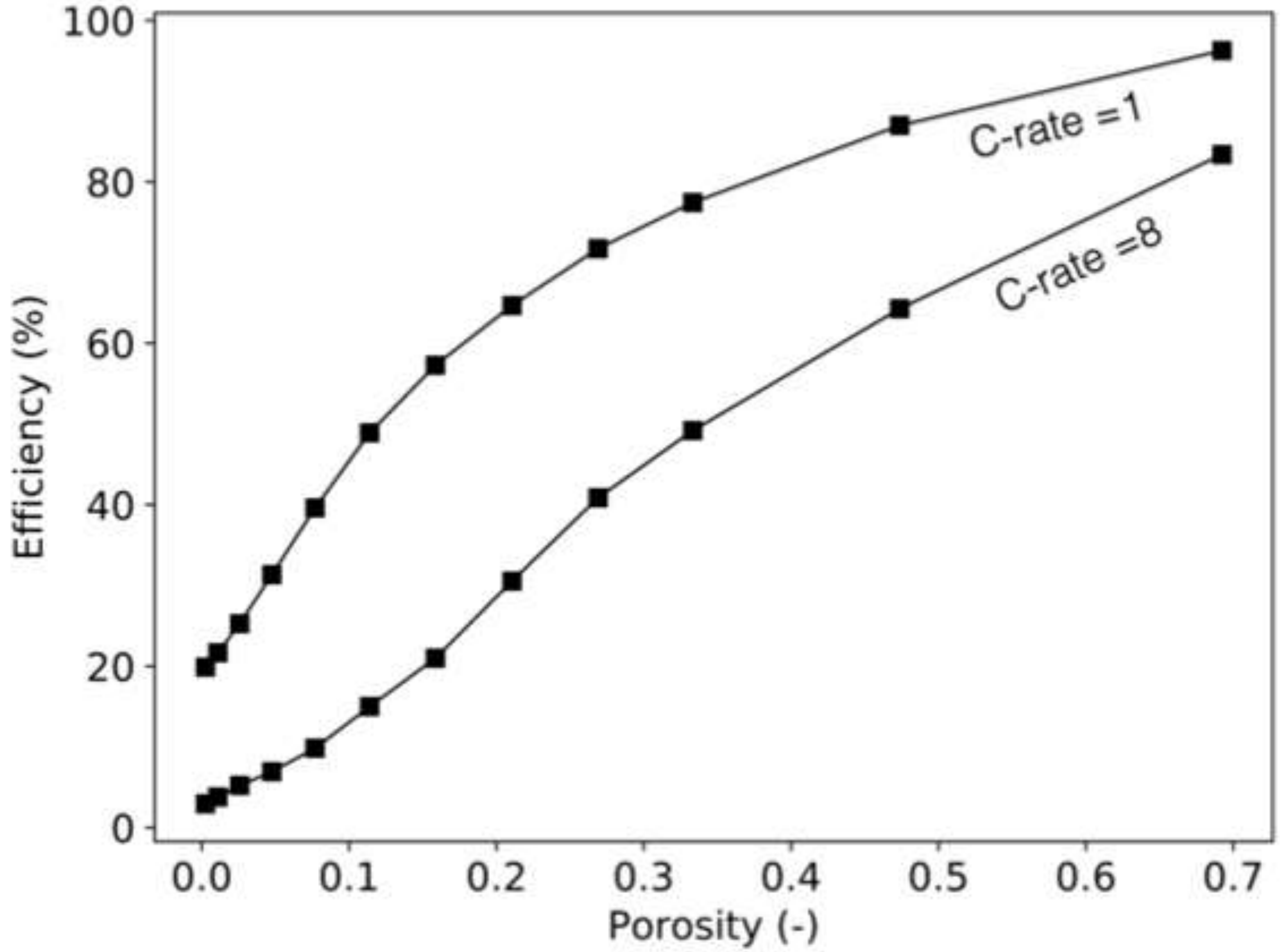


Figure 13: *Impact of battery morphology on the simulated voltage for 1.0 (a) and 8.0 (b) C-rate discharging. Each voltage profile is labeled by the integer n, i.e. the constant that identifies the shape of the electrodes (see Fig. 4). The battery efficiency, reported in parenthesis, is computed as the ratio between the extracted charge at the end of the discharging and the theoretical capacity.*

Shape optimization for electrodes



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Conclusions