northvolt®

# Multiscale Methodologies for Electrolyte Characterization

ENCCS Industry Days 2022

*Matteo Ambrosetti – Advanced Material Engineer*

# Introducing Northvolt

Founded in 2016, Northvolt aims to become Europe’s leading supplier of sustainable, high-quality battery cells and systems.


No other battery company holds as high a commitment to developing green, sustainably sourced and manufactured batteries.

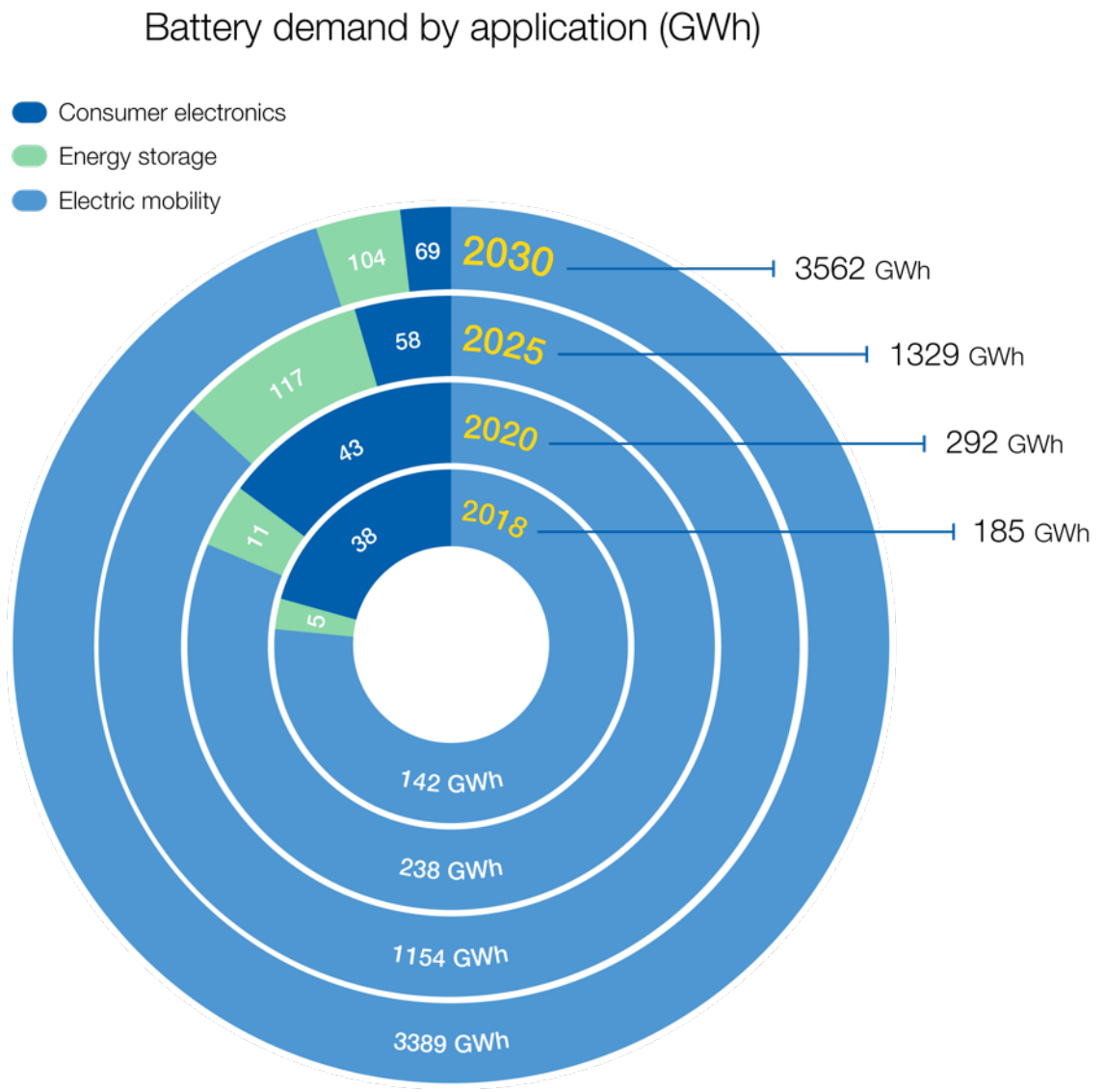
northvolt

# Accelerating demand

While lithium-ion batteries are key to a clean future, we face a great shortfall in supply.

Especially in Europe, where we have little domestic manufacturing capacity.

We’re currently in the middle of a global ramp-up in battery manufacturing capacity to meet this demand.

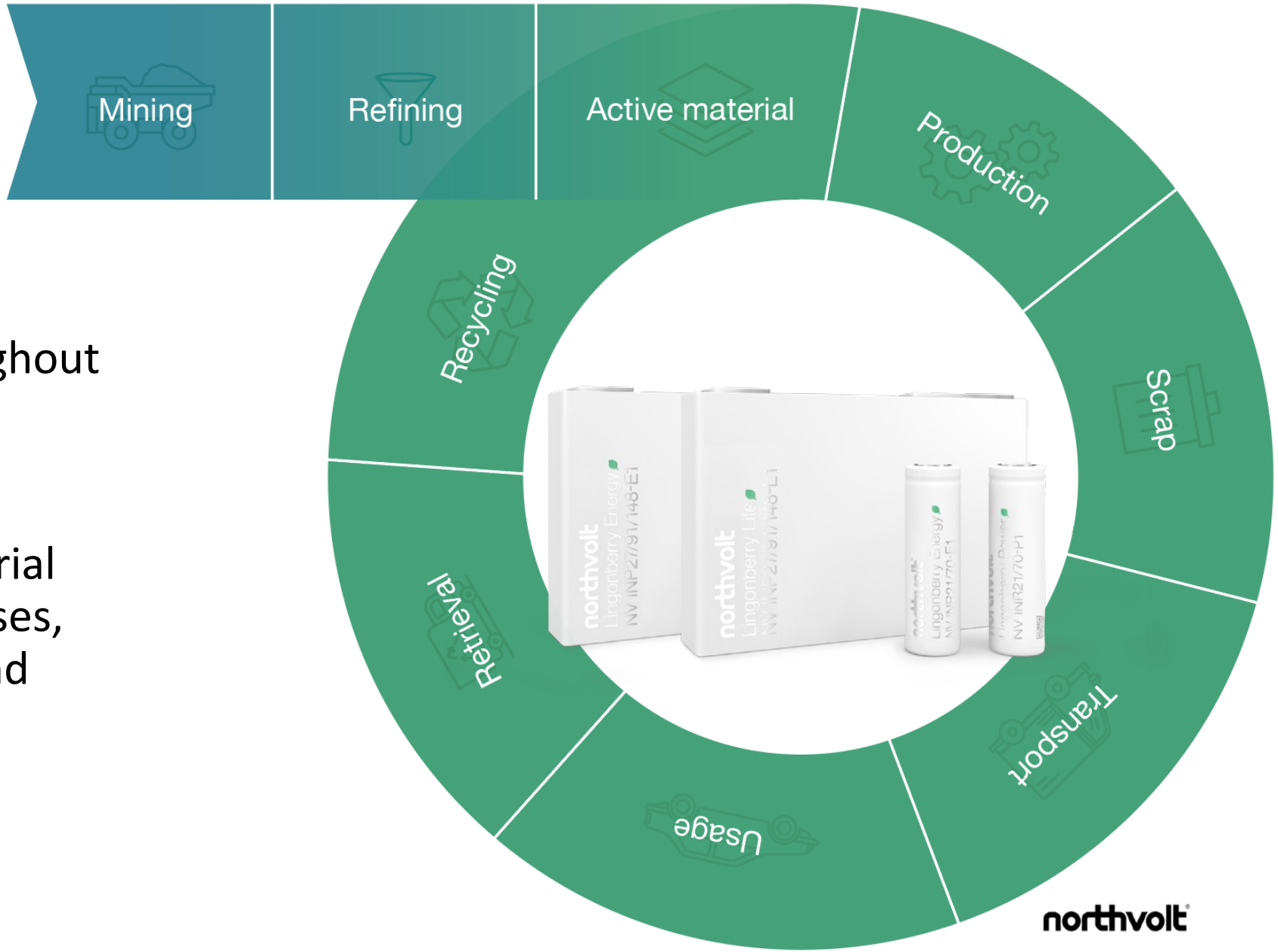



Public

# The Northvolt loop

Northvolt's commitment to sustainability extends throughout the battery supply chain.

Focus is placed on raw material sourcing, production processes, logistics, battery recovery and recycling.




© 2020 Northvolt AB / Public / Non-NDA

northvolt

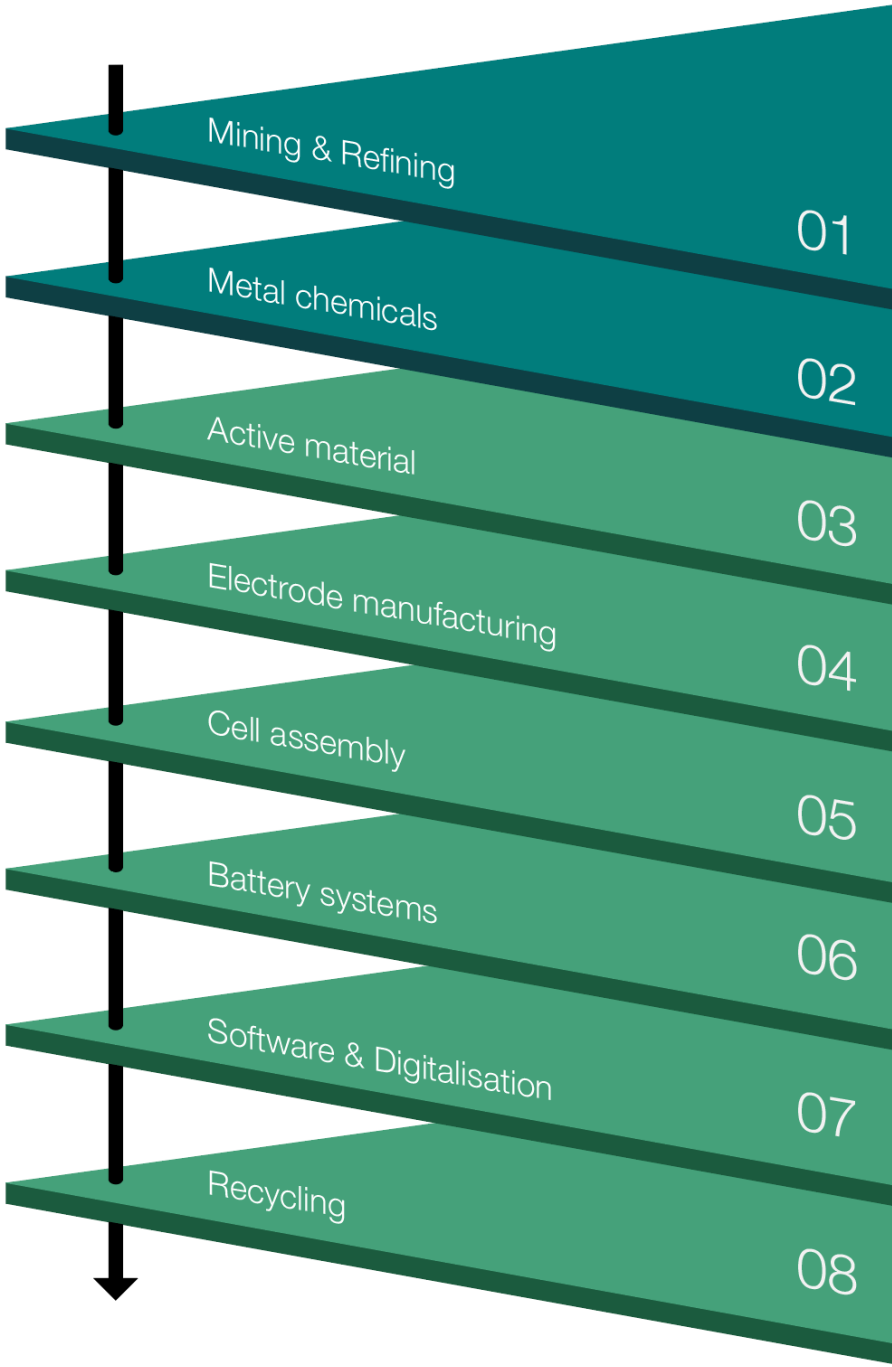
Public

# Vertical integration

The model adopted by Northvolt involves bringing as much of the supply chain in house as possible.

Critically, this involves in-house upstream manufacturing of active material used in cathode electrode production.

Northvolt capacities extend downstream, with battery systems development, digitalization and recycling.




© 2020 Northvolt AB / Public / Non-NDA

Public

## Labs

Research & development and manufacturing hub for industrialization of cell products, processes and batteries.

## Ett

Northvolt’s first gigafactory. Features upstream and downstream production, along with recycling.

## Systems

Assembly plant for battery modules and energy storage systems for grid and industry.

northvolt

# **Northvolt** Labs

A springboard to larger cell production gigafactories.

A base of operations for cell industrialization.

A platform for R&D and innovation.

**Västerås,** Sweden

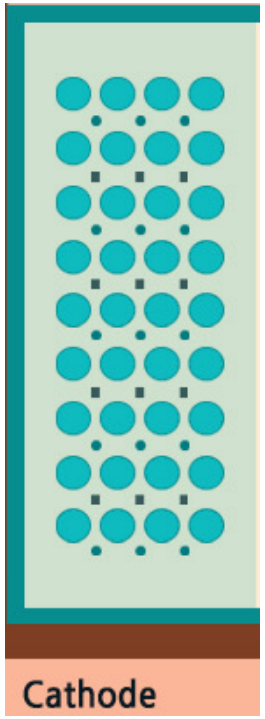

Public

# The Advanced material team



Public

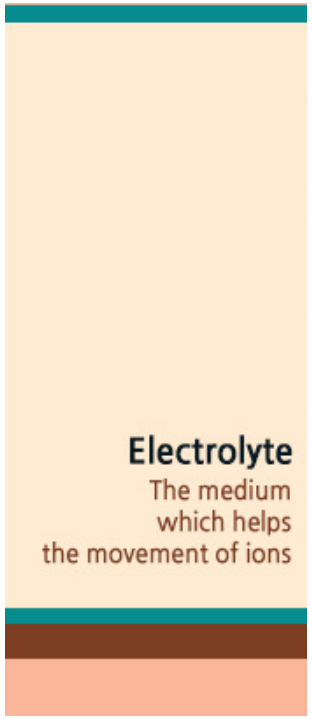
# Battery components






Public

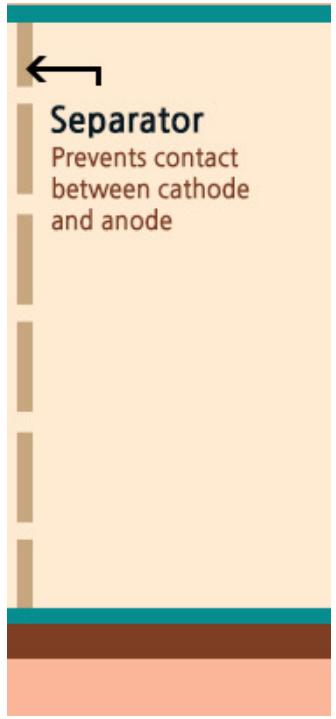
# Battery components






Public

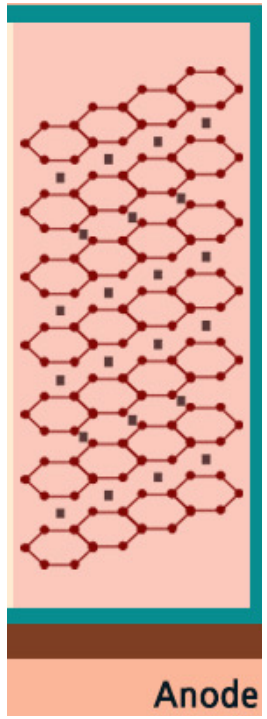
# Battery components






Public

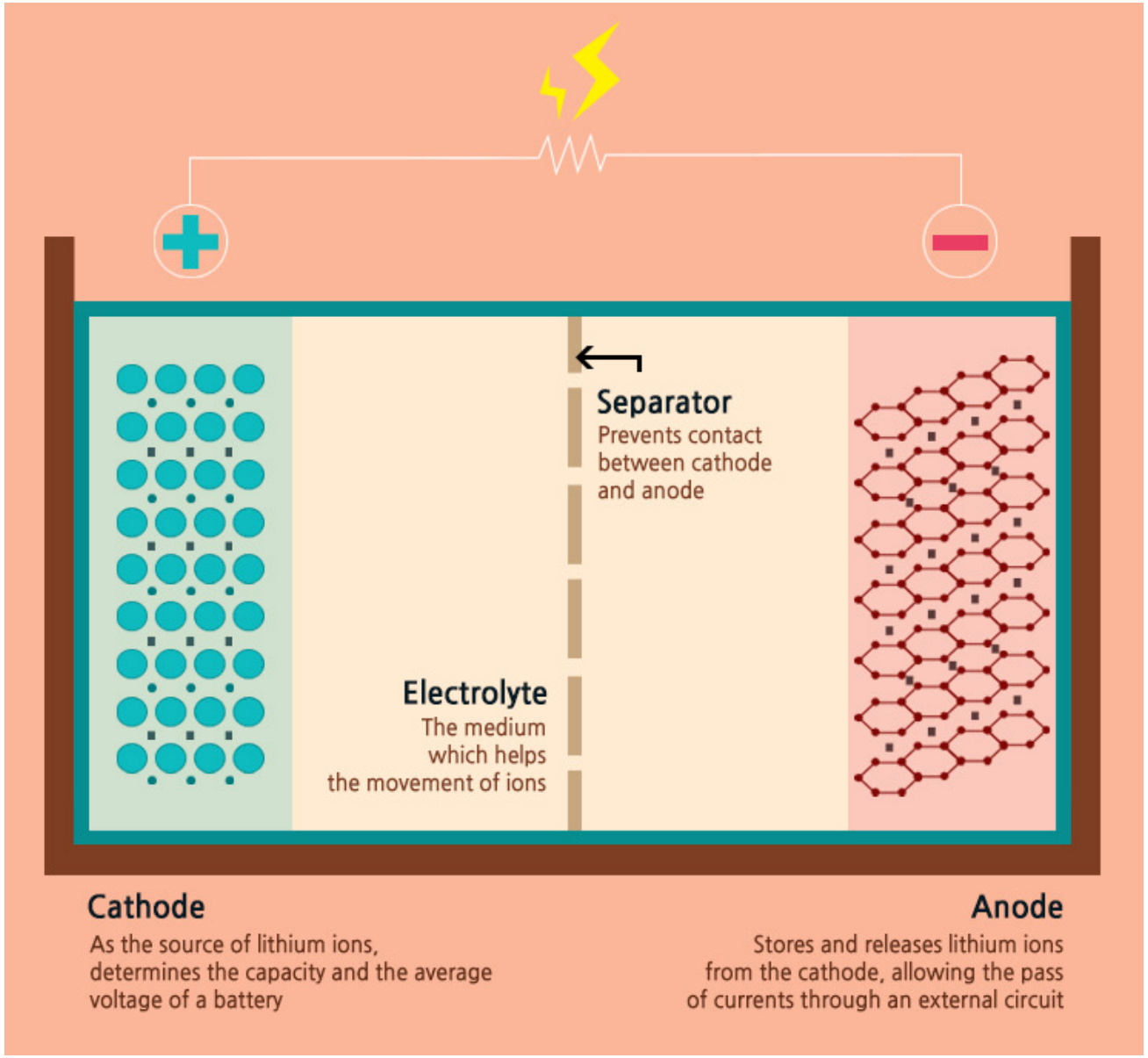
# Battery components






Public

# Battery components

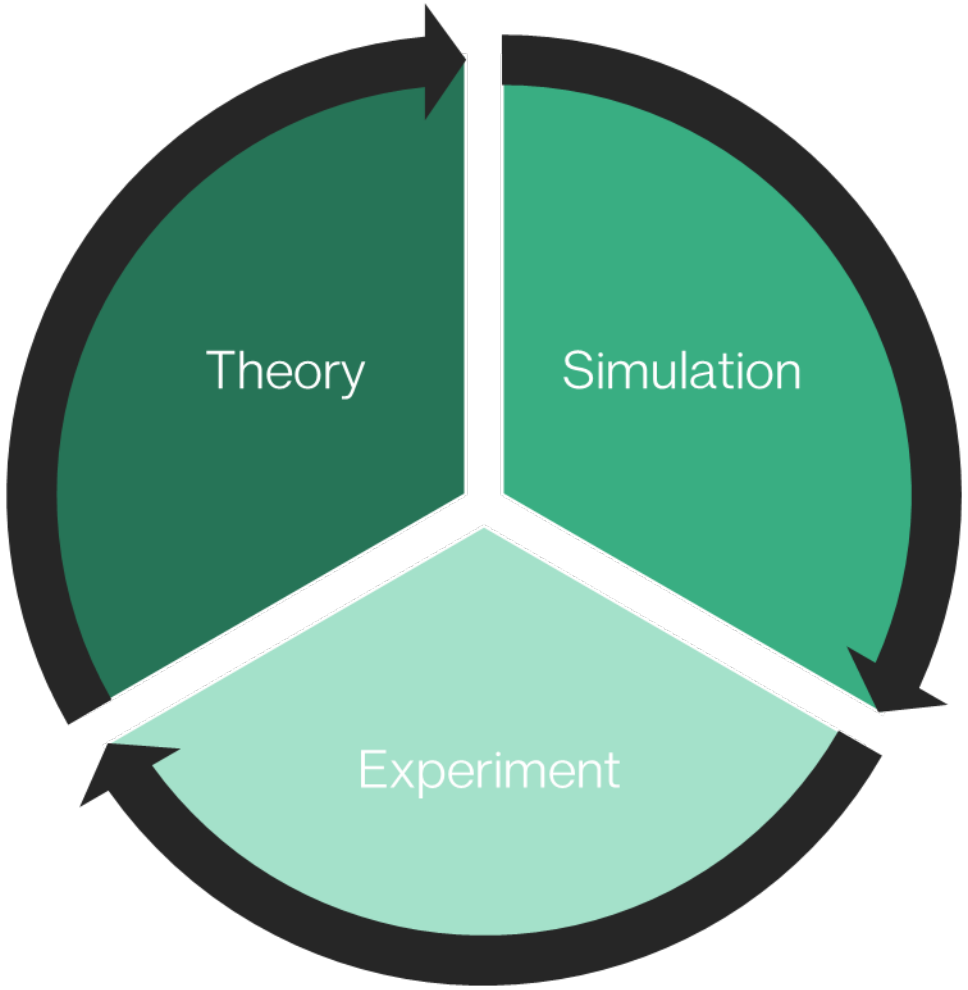



Source: The Four Components of a Li-ion Battery (samsungsdi.com)



Public

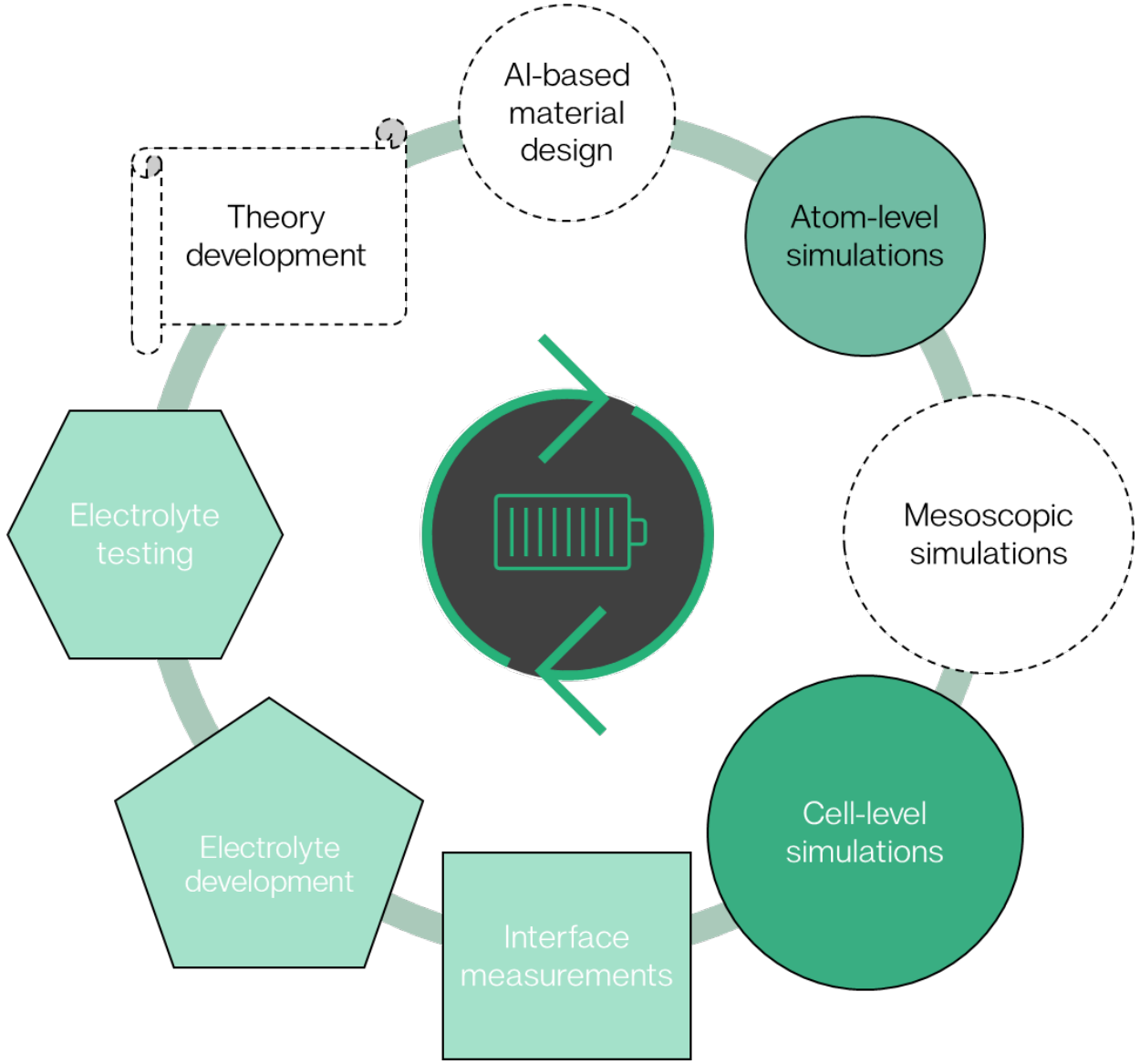
# Research & Development workflow






Public

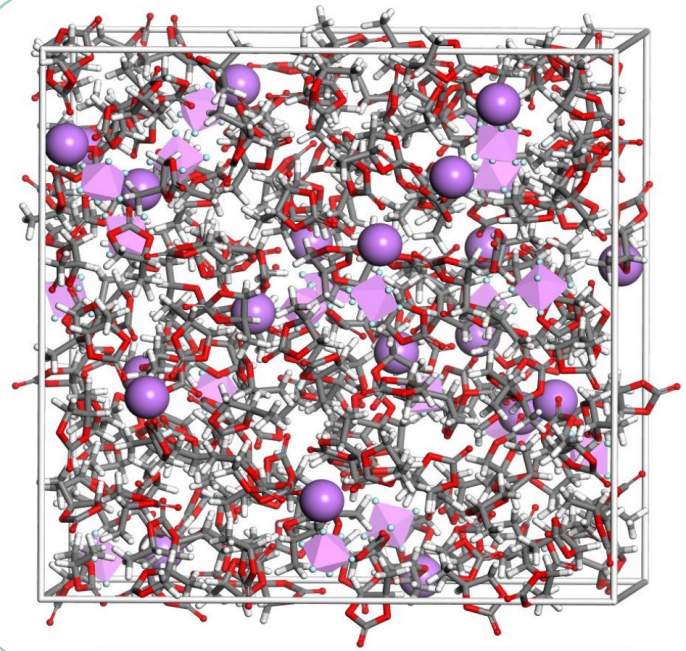
# Research & Development advanced workflow






Public

# Single Component



Electrolyte

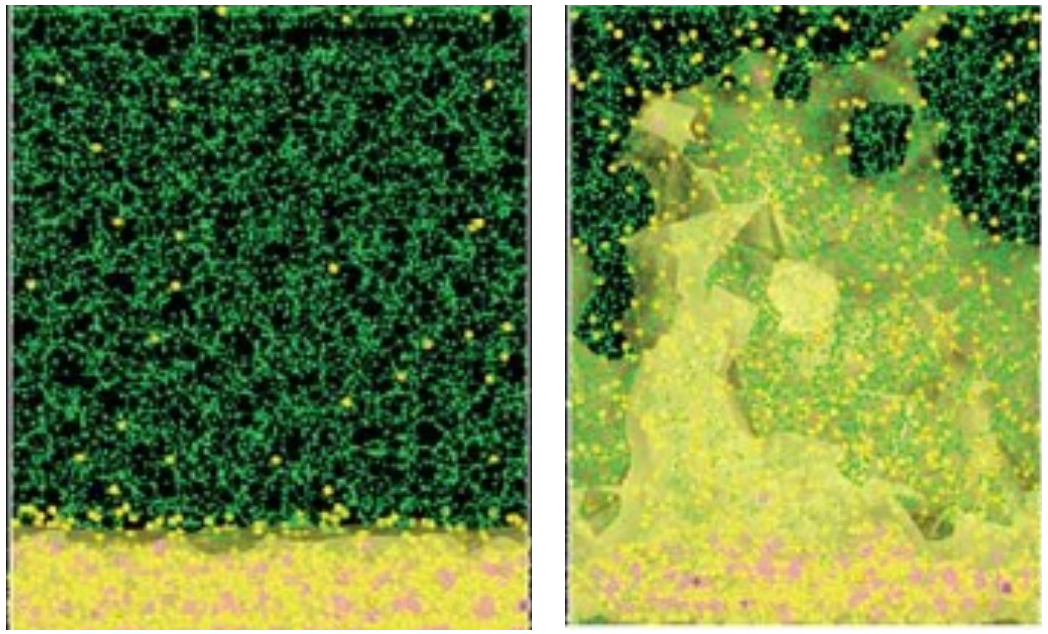
*Nat. Mater.* **19**, 1339–1345

Electrode



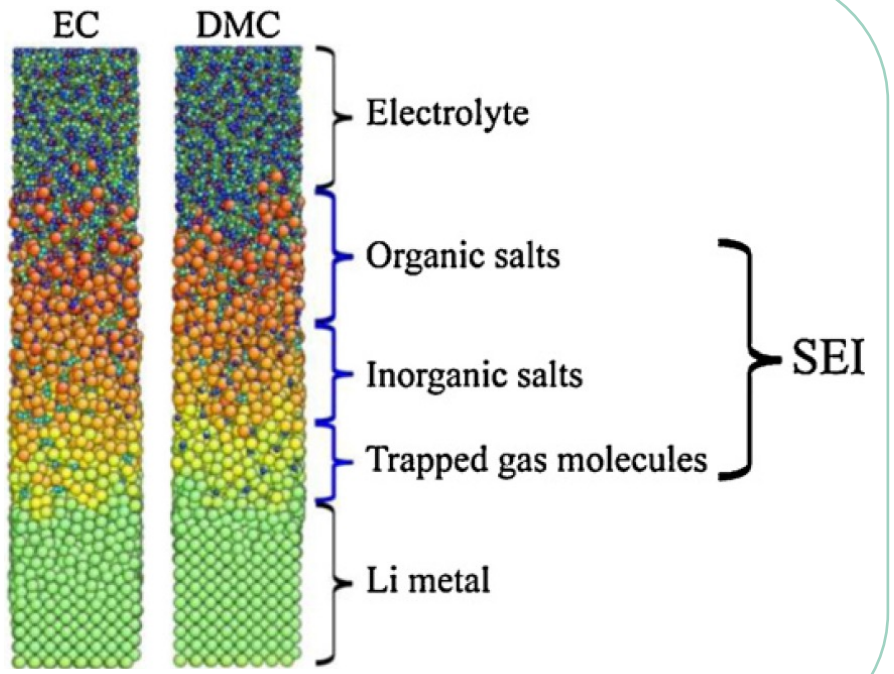
Public

# Interfaces



RSC Adv., 2018, **8**, 5255-5267

Dendrites



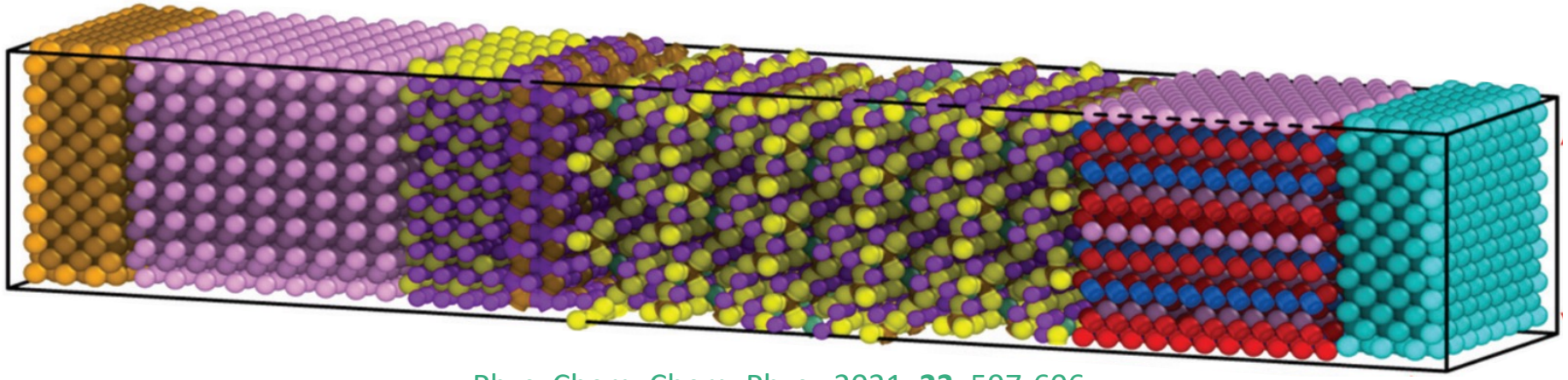

*J. Phys. Chem. C* 2018, 122, 20, 10783–10791

SEI/CEI



Public

# Nanobattery



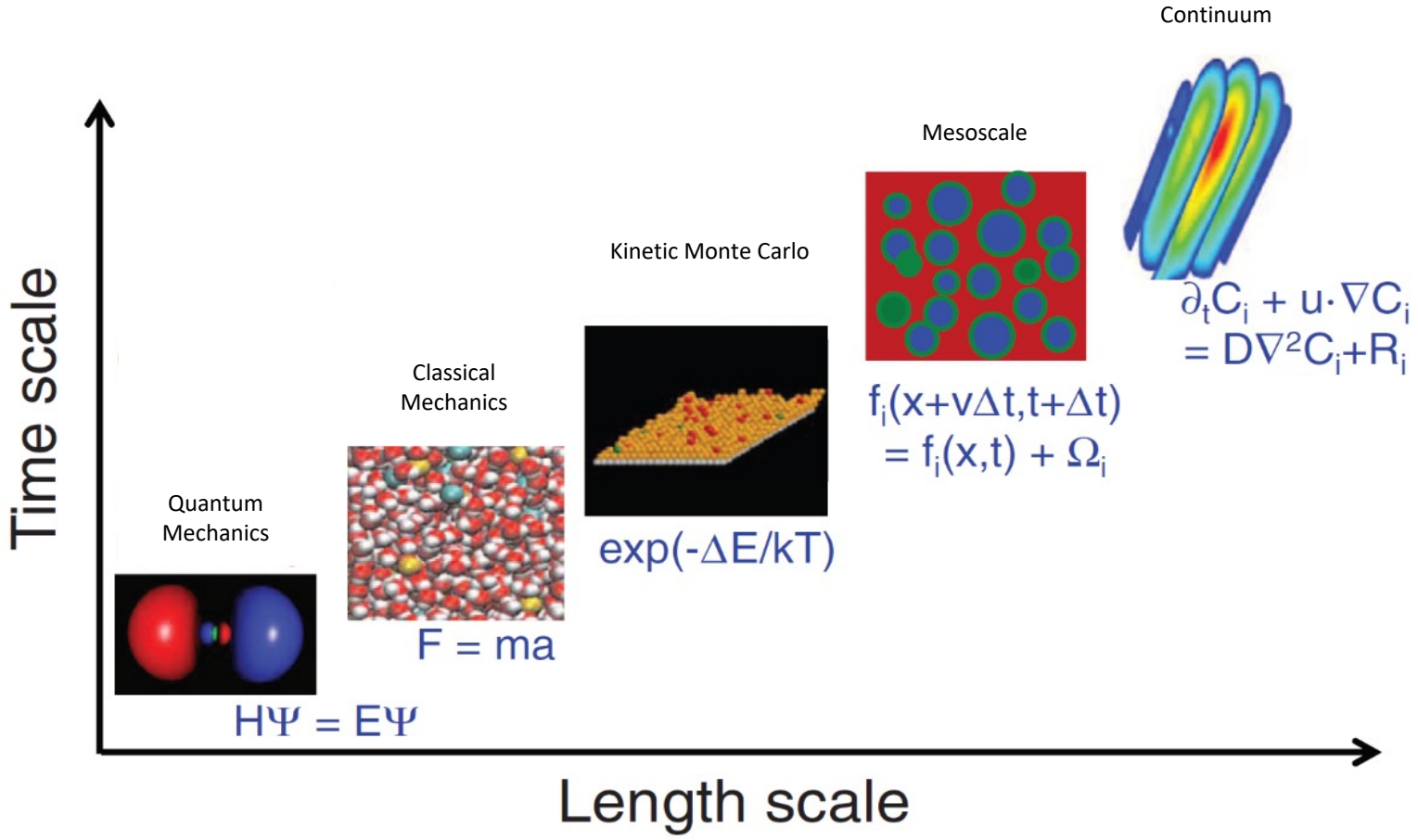
Phys. Chem. Chem. Phys., 2021, **23**, 597-606

Complete system



Public

# Multiscale approach

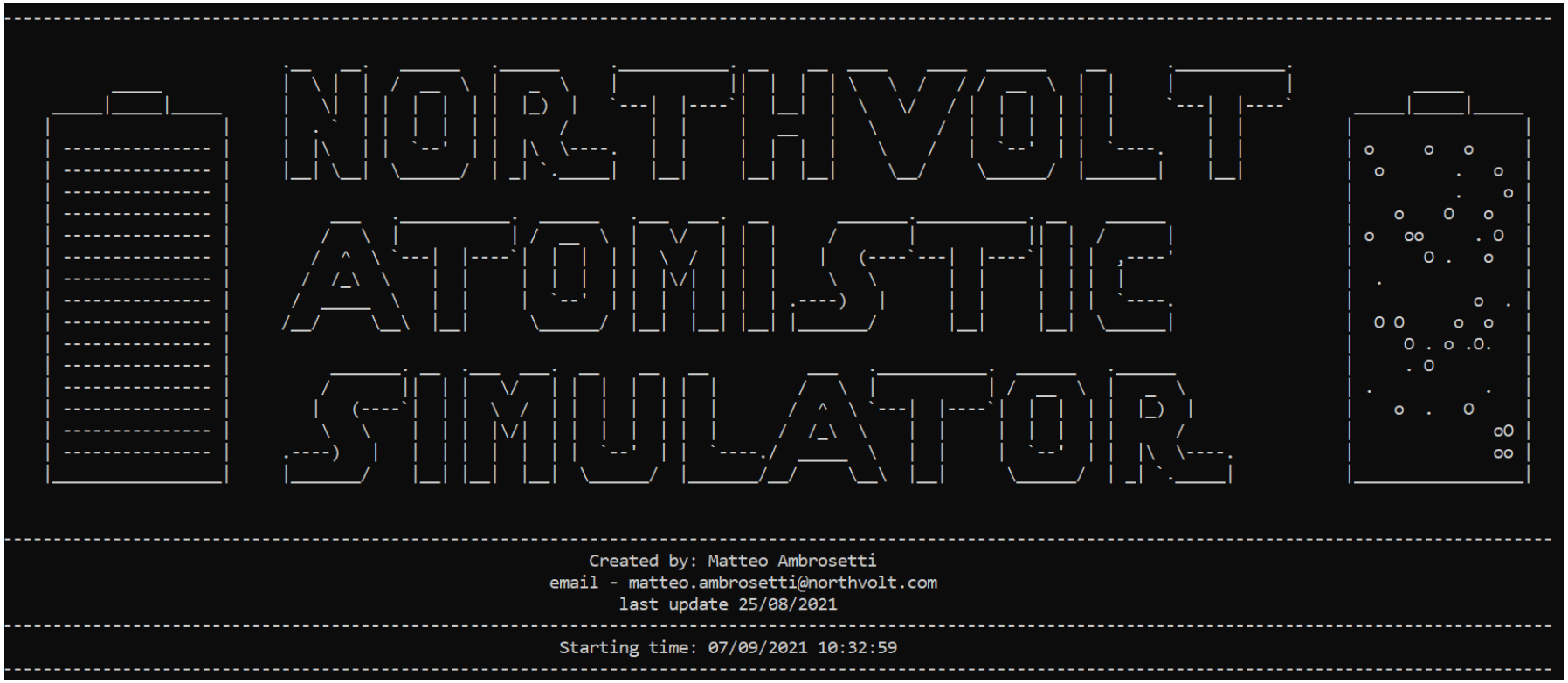



Different phenomena are observed at different length and time scales



Public

# In-house software development




| Advantages | Disadvantages |
|---|---|
| Highly customizable | In some case reinvent the wheel |
| We know what is happening under the hood | Validation can be time consuming |
| Cheaper than licensed software | No GUI |
| Interface easily with other tools | Not optimized |



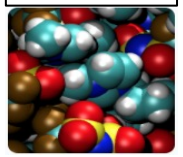
Public

# In-house software development – under the hood

**Literature/LigParGen**


Force Field assignment (OPLS-AA)

**fftool**



Force Field conversion (OPLS-AA)

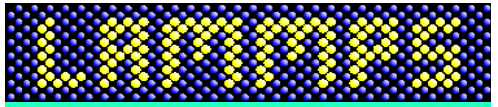
**Packmol**

Initial configuration

**Northvolt Atomistic Simulator**

Wrap all

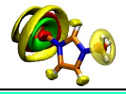
- Electrolyte database
- System composition
- Charge scaling
- LAMMPS input
- Trajectory conversion
- Plot results
- Custom analysis



Molecular Dynamics

- Classical
- Polarizable / Reactive (TBI)
- Liquid systems (NPT, NVT, NVE)

**TRAVIS**
Trajectory Analyzer and Visualizer



**PyLAT**

Analysis tool

- Diffusion coefficient
- Conductivity (NE & GK)
- Viscosity
- Dielectric constant
- Molecule pair lifetime
- Radial distribution function
- Coordination number
- Cluster extraction
- Contact matrix
- Velocity autocorrelation function
- Plane projection distribution
- …



Public

# Molecular Dynamics – a soft introduction

$$\boldsymbol{F} = m \cdot \boldsymbol{a}$$

$$\boldsymbol{F} = -\boldsymbol{\nabla} U$$

Each atom composing the system is described by a set of parameters which takes the name of Force Field.
There are several Force Fields that can be used for a specific problem depending on the desired observables/properties:

- Non-reactive (e.g., UFF, OPLS, AMBER, CHARMM, …)
- Polarizable (e.g., AMBER, AMOEBA, APPLE&P, …)
- Reactive (e.g., ReaxFF, …)

$$U^{OPLS} = U_{bonded} + U_{nonbonded}$$

Intramolecular interactions

Intermolecular interactions

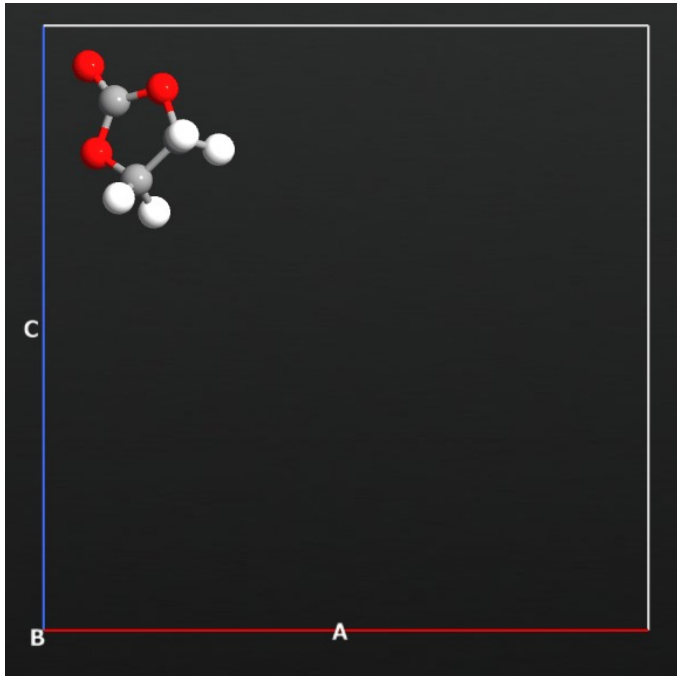


Public

# Molecular Dynamics – 1 EC @ 300K NVT 1ps Δt=2fs

$$U_{bonded} = U_{bonds} + U_{angles} + U_{dihedrals}$$

$$U_{bonds} = \sum_{bonds} k_r(r - r_0)^2$$



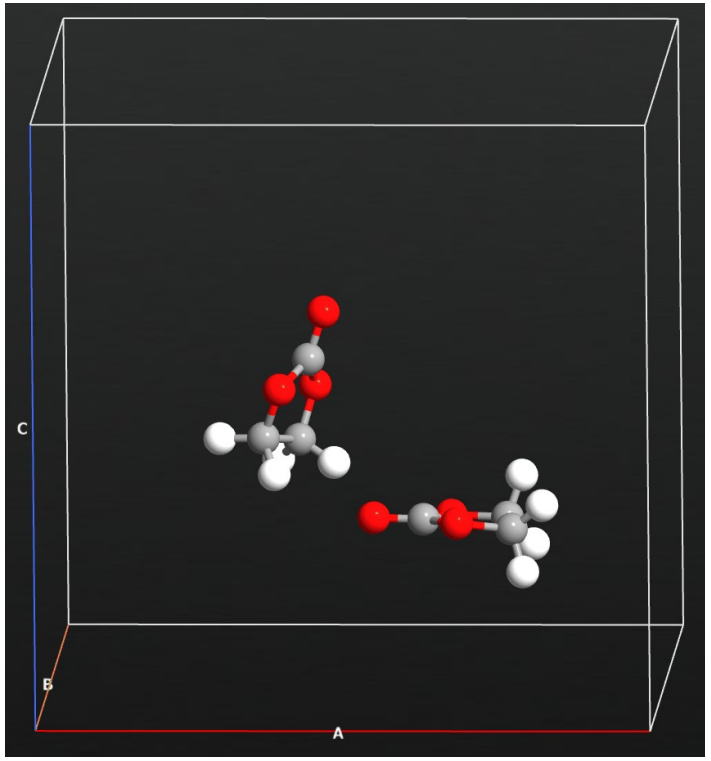



Public

# Molecular Dynamics – 2 EC @ 300K NVT 1ps Δt=2fs

$$U_{bonded} = U_{bonds} + U_{angles} + U_{dihedrals}$$

$$U_{nonbonded} = U_{vdW} + U_{Coulomb}$$



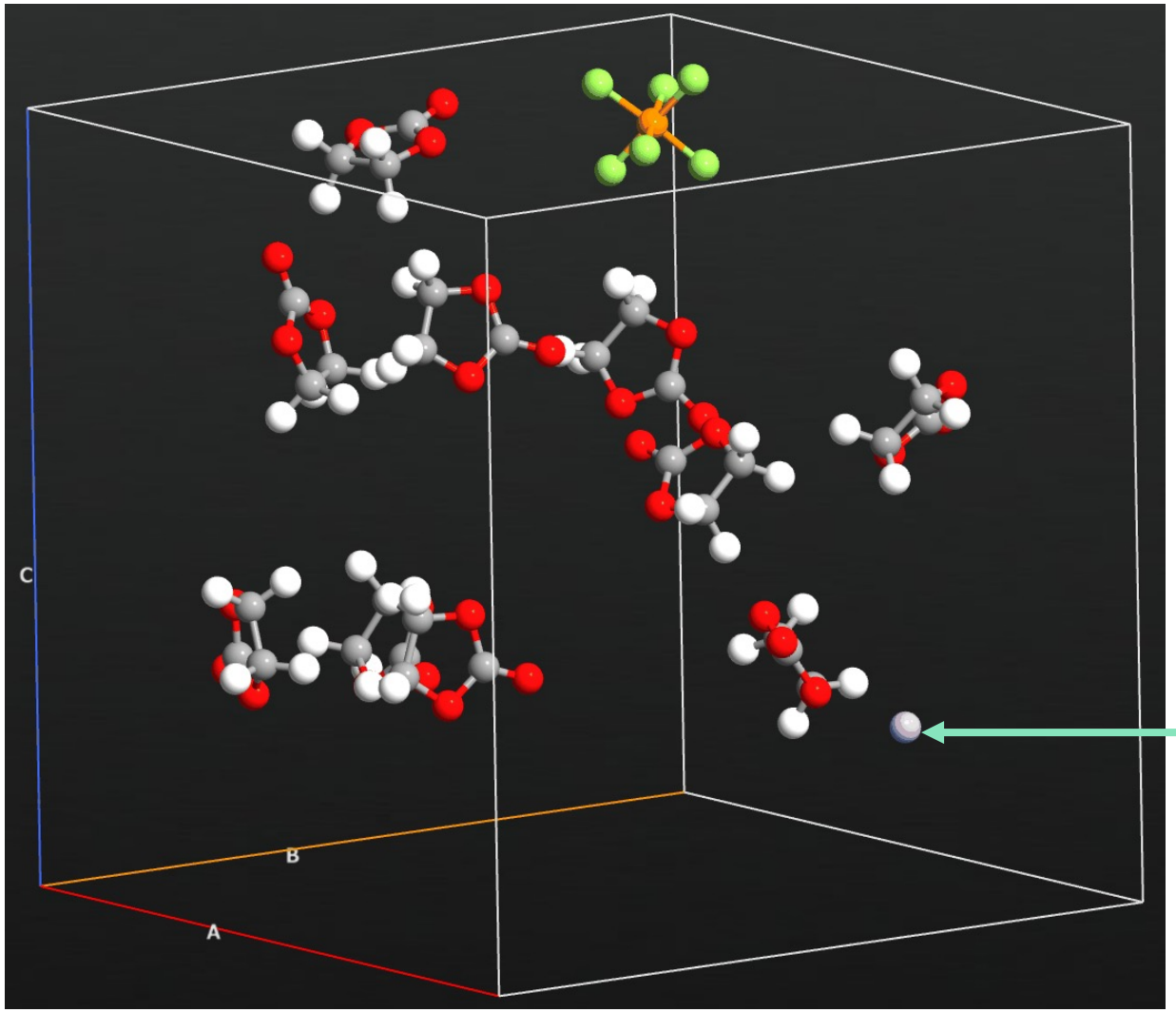



Public

# Molecular Dynamics – 10 EC + 1 $LiPF_6$ @ 300K NVT 1ps Δt=2fs

Properties of interest:

- Diffusion coefficient
- Transference number
- Solvation structures
- Diffusion mechanism
- Ionic conductivity
- Reactivity
- Density
- Viscosity
- Coordination number
- Charge distribution
- …



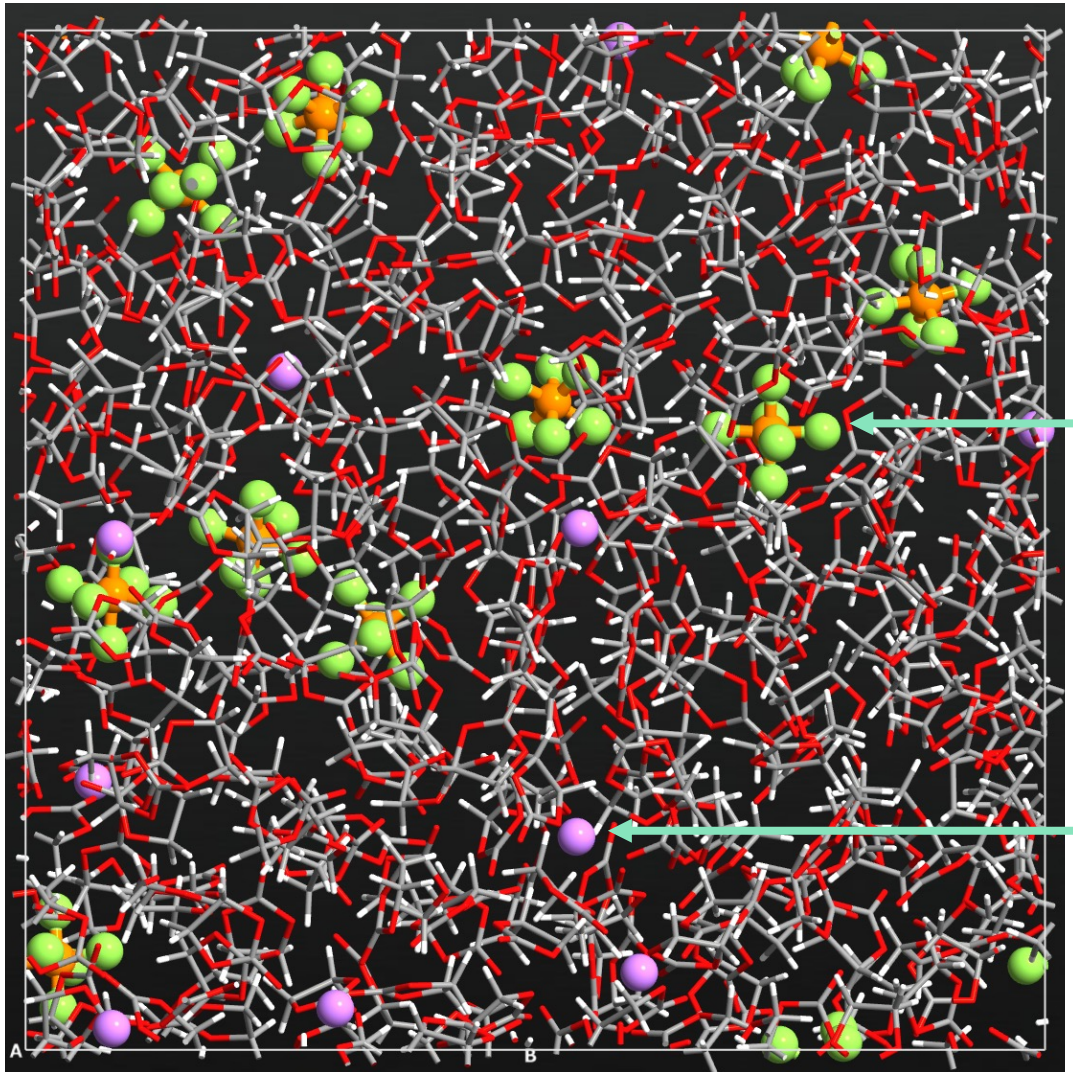



Public

# Molecular Dynamics – 300 EC + 10 $LiPF_6$ @ 300K NPT 10ns Δt=2fs

Properties of interest:

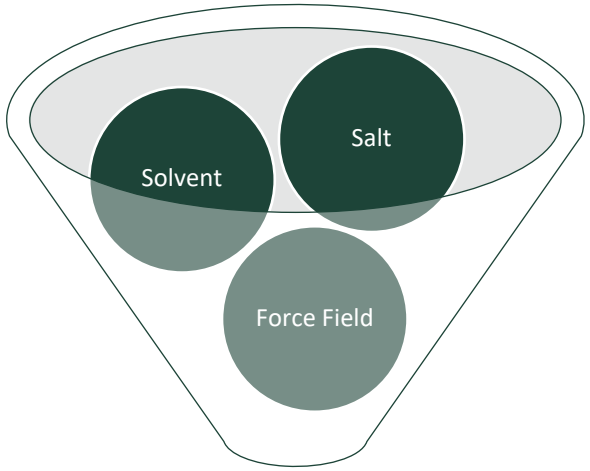
- Diffusion coefficient
- Transference number
- Solvation structures
- Diffusion mechanism
- Ionic conductivity
- Reactivity
- Density
- Viscosity
- Coordination number
- Charge distribution
- …





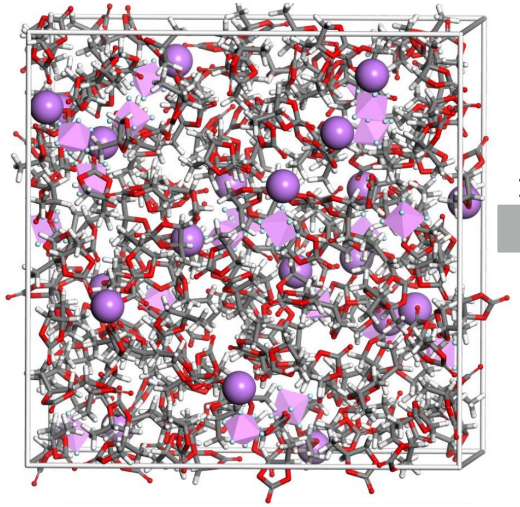

Public

# Multiscale approach – bottom-up

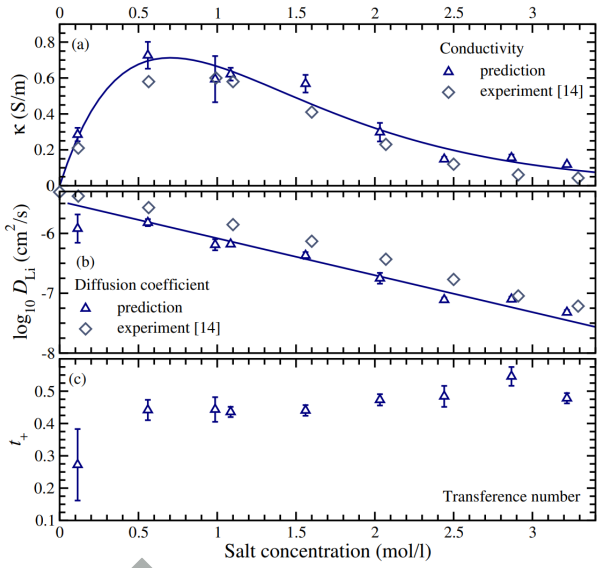



200 EC + x($Li^+PF_6^-$)

x = salt concentration (variable)



100 ps NPT
+
5 ns NVE

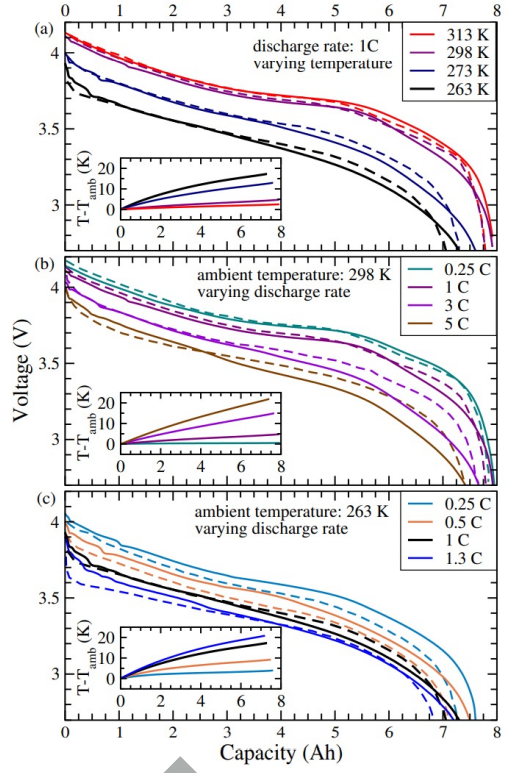



Nerst-Einstein equation

$\kappa_i = D_i c_i e^2 N_A (k_B T)^{-1}$

- $\kappa_i$ Ionic conductivity
- $D_i$ Salt diffusion coefficient
- $t_i$ Transference number

$i = Li^+/PF_6^-$

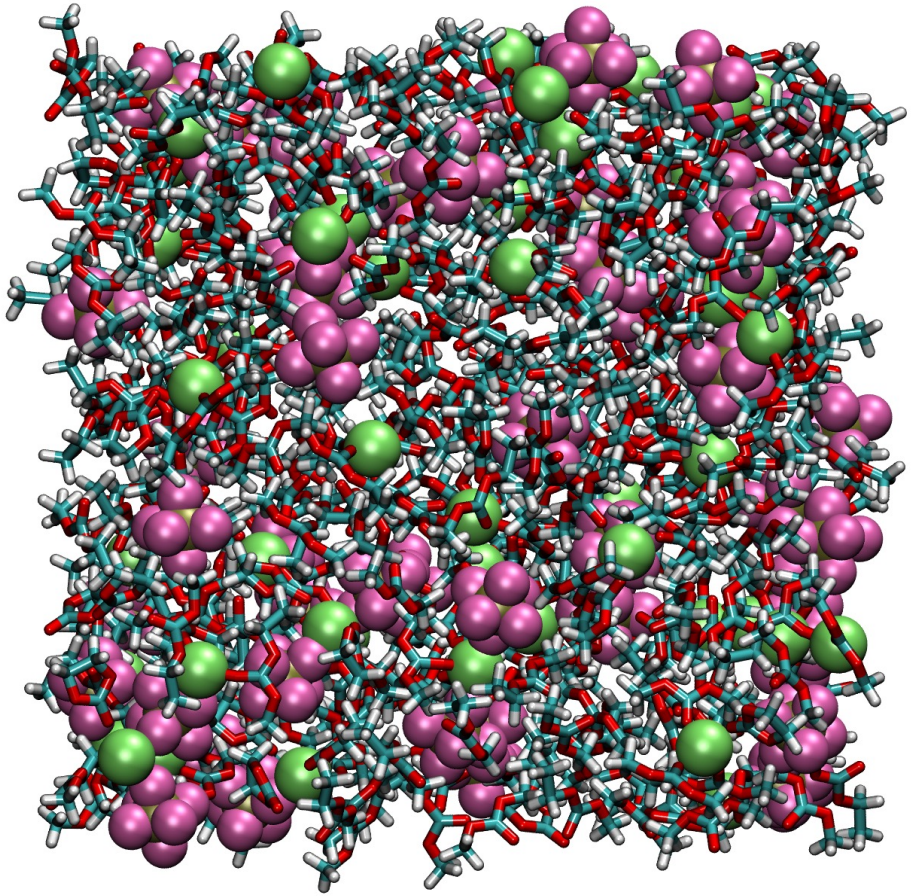



Pseudo two-dimensional electrochemical Newman model



Public

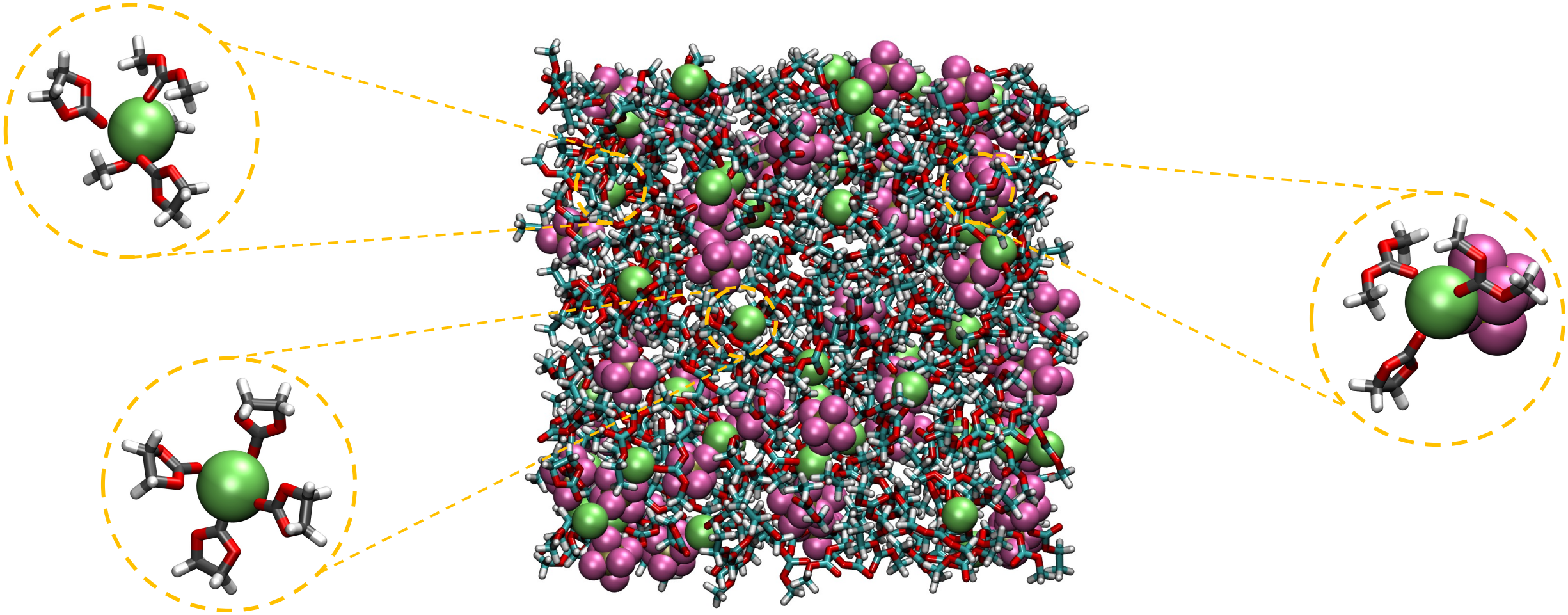
# Electrolyte system – top-down





Public

# Electrolyte system – top-down

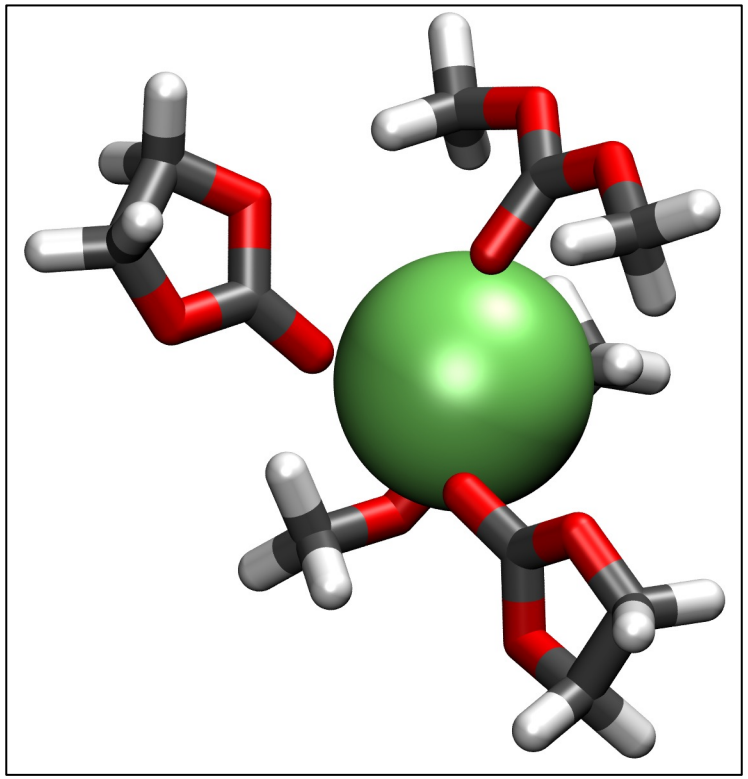




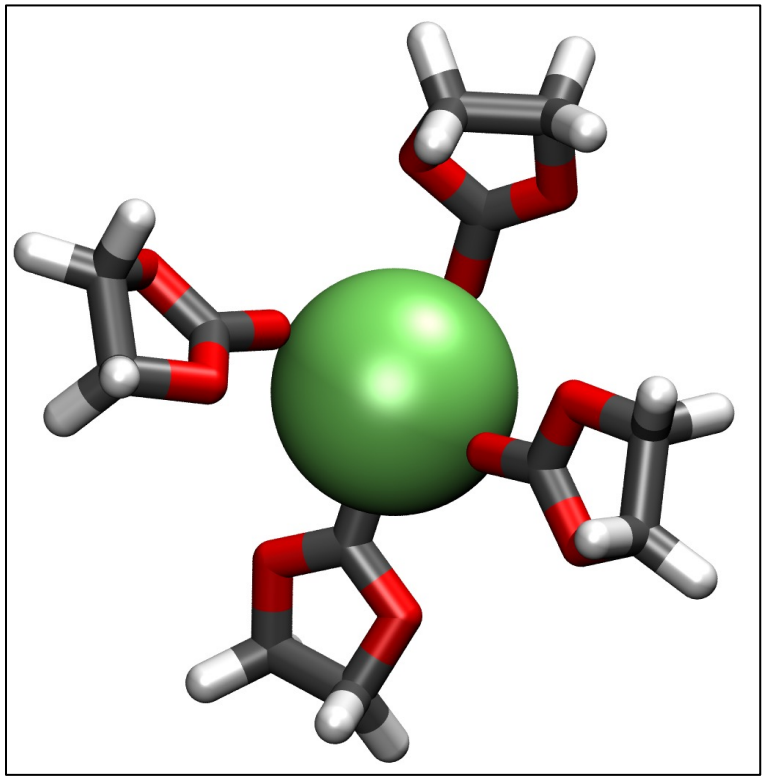
Public

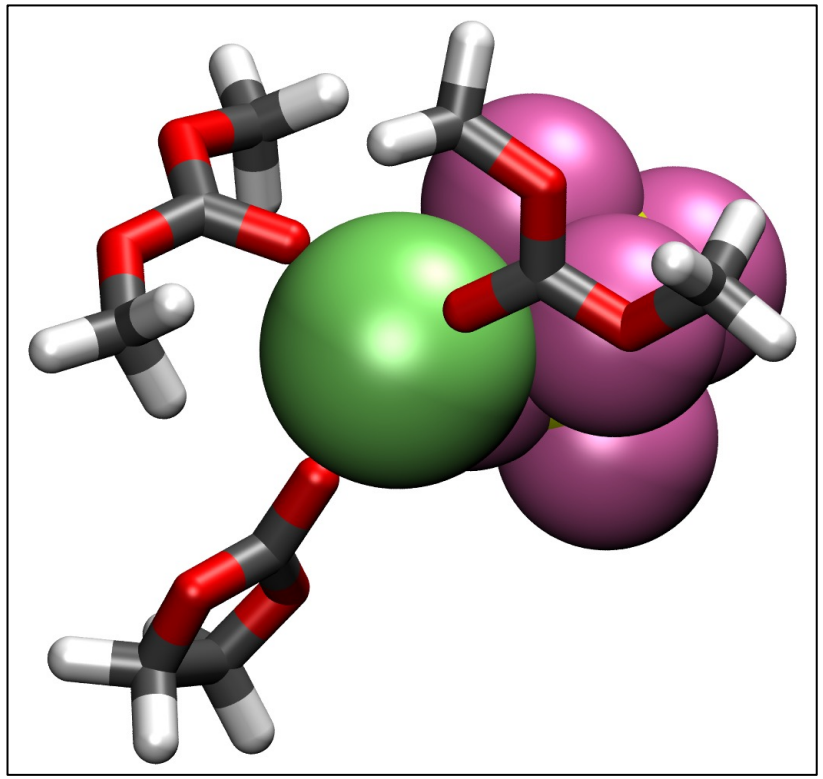
# Electrolyte system – top-down

$Li^+$ coordination shell



Less stable structure





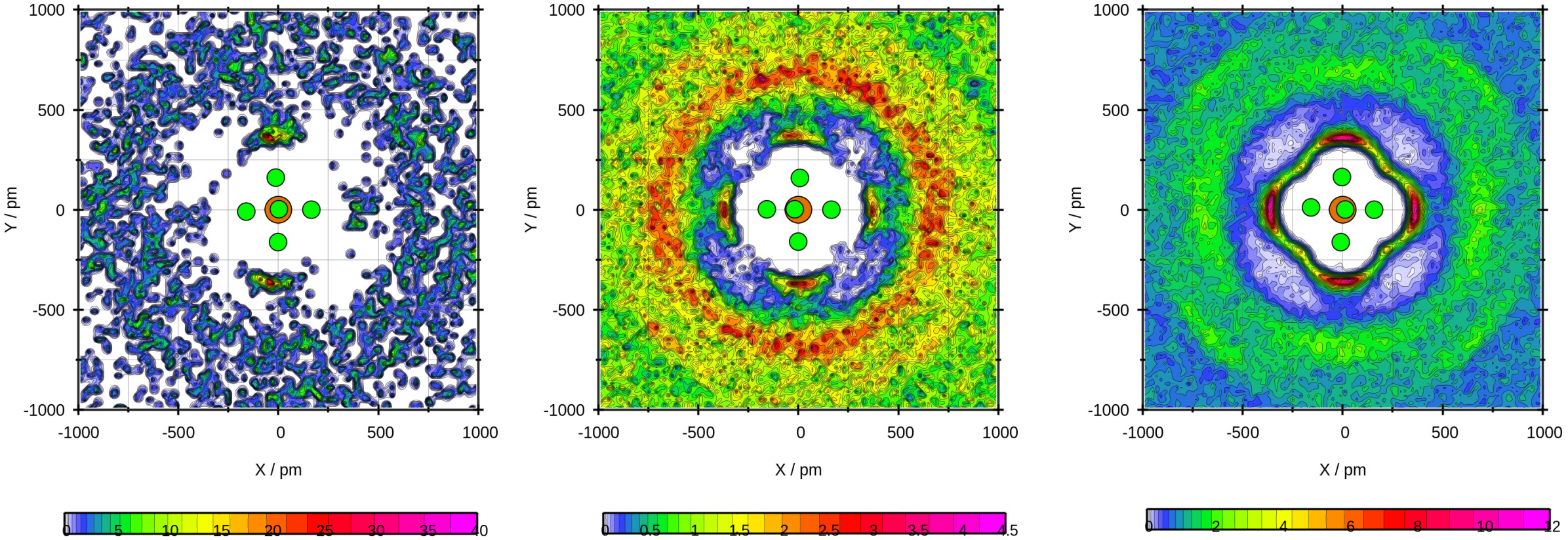
More stable structure



Public

# Electrolyte system – global properties

Probability of finding a $Li^+$ atom around a $PF_6^-$ molecule



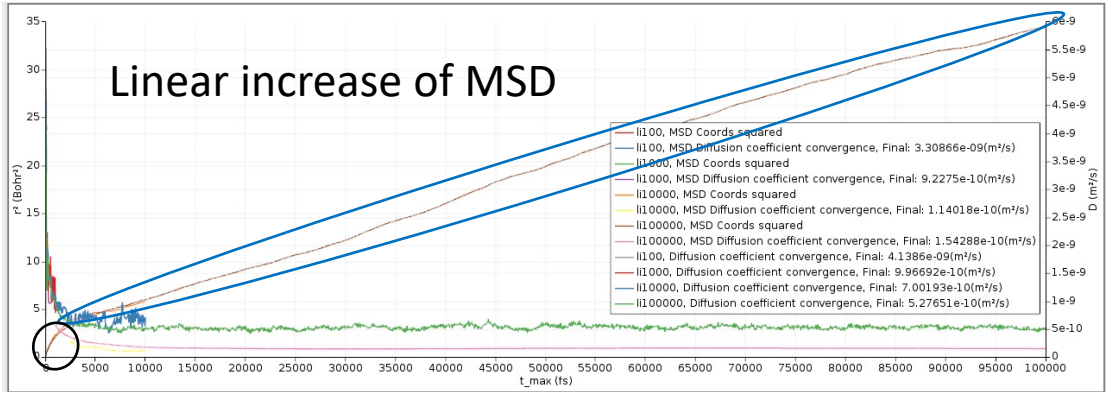

Salt concentration



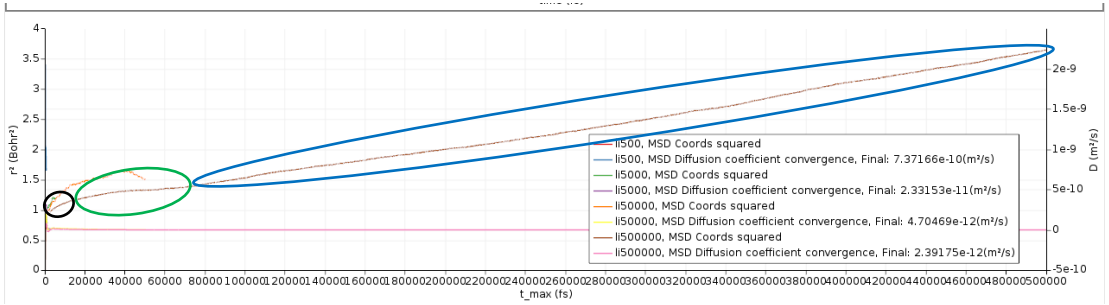
Public

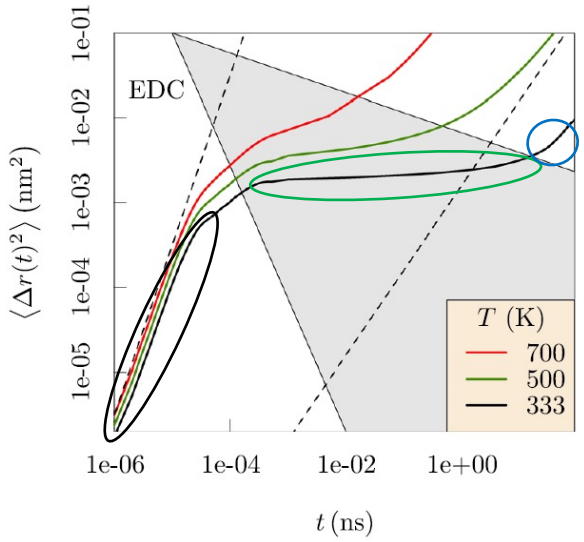
# Electrolyte system – global properties

## Low concentration




## High concentration

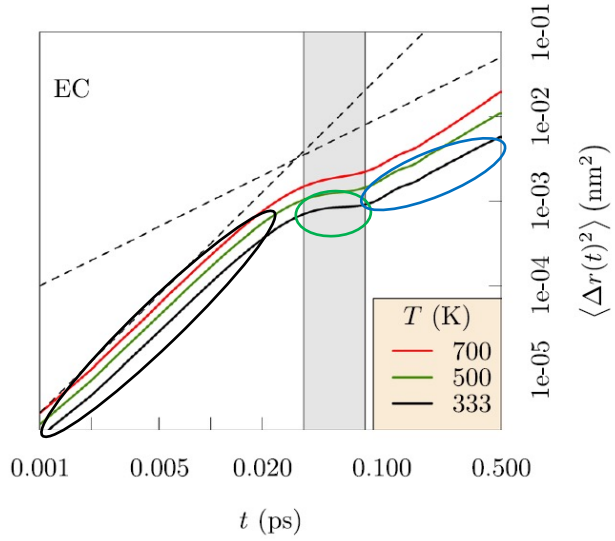



Ballistic regime

Trapping regime

Diffusive motion

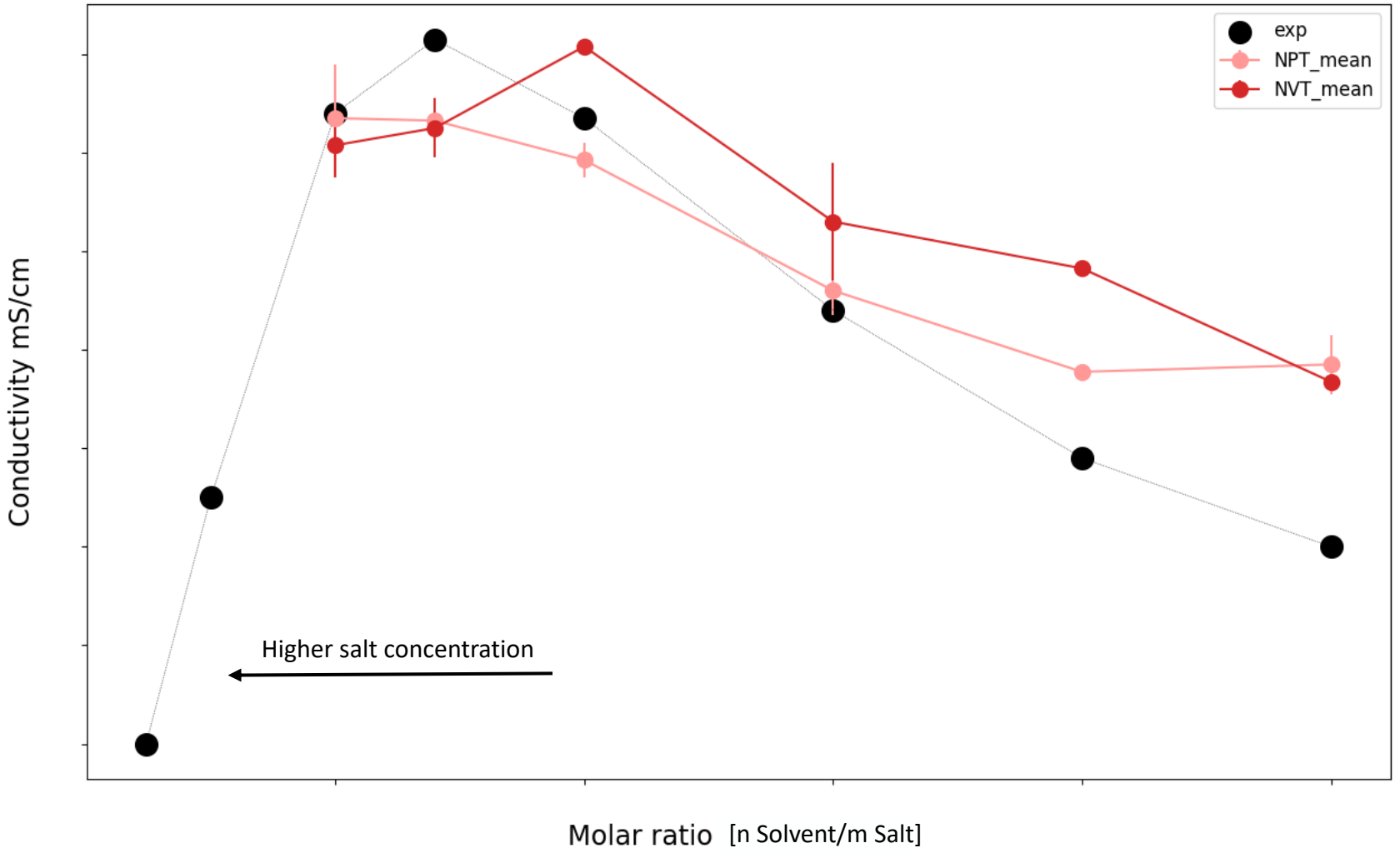



(2018) 8:10736 | DOI:10.1038/s41598-018-28869-x


© 2021 Northvolt AB, Strictly Confidential

Confidential

# Electrolyte – Salt concentration optimization



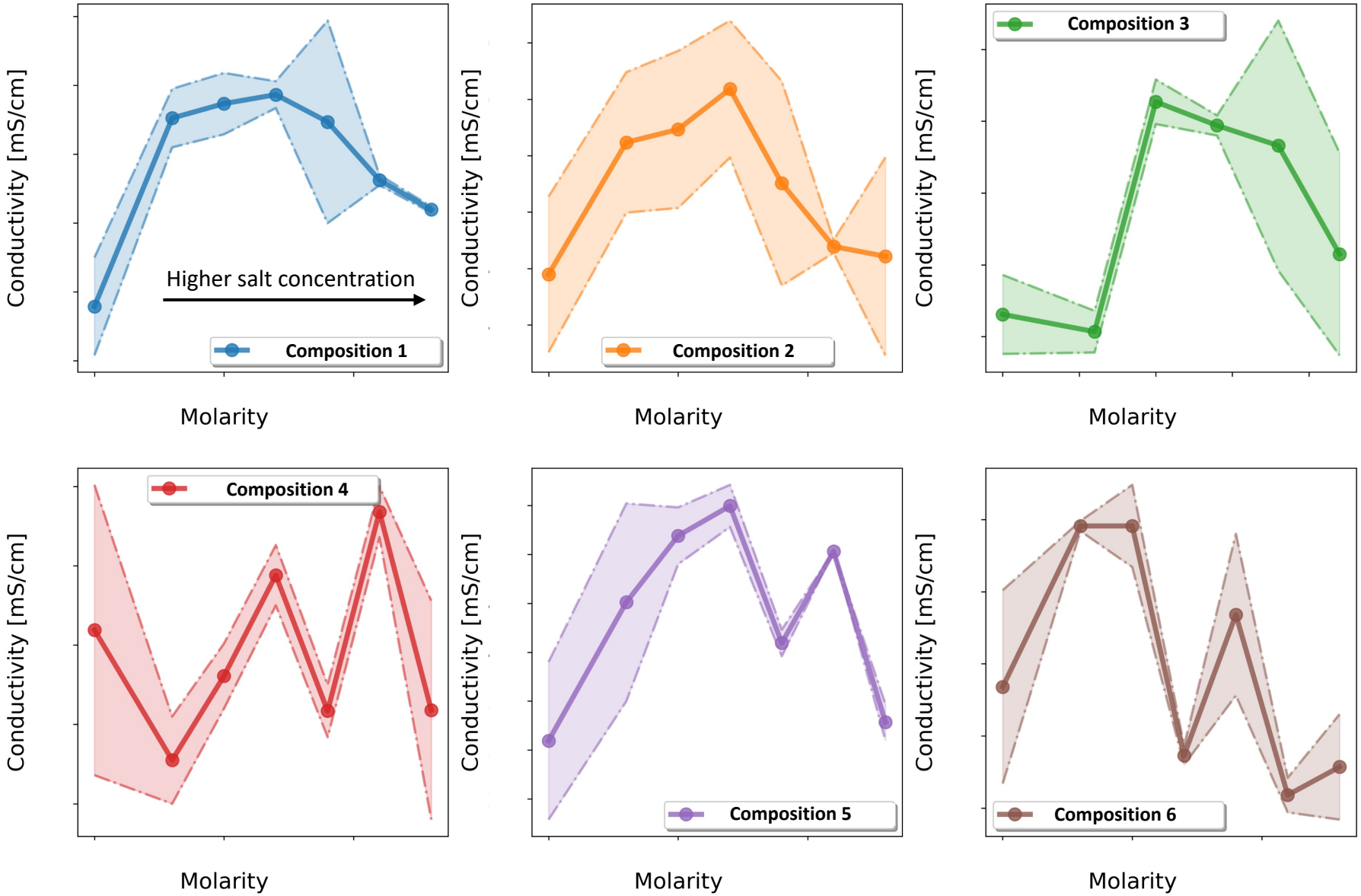

- Composition of the system:
  - 600 Solvent + x Salt (x = 24-500)
- Ensemble:
  - NVT
  - NPT
- Simulation length: 10 ns
- Total number of simulations:
  - 24

*Results scaled by conductivity minimum in order to evidence relative variation



Public

# Electrolyte – Composition optimization

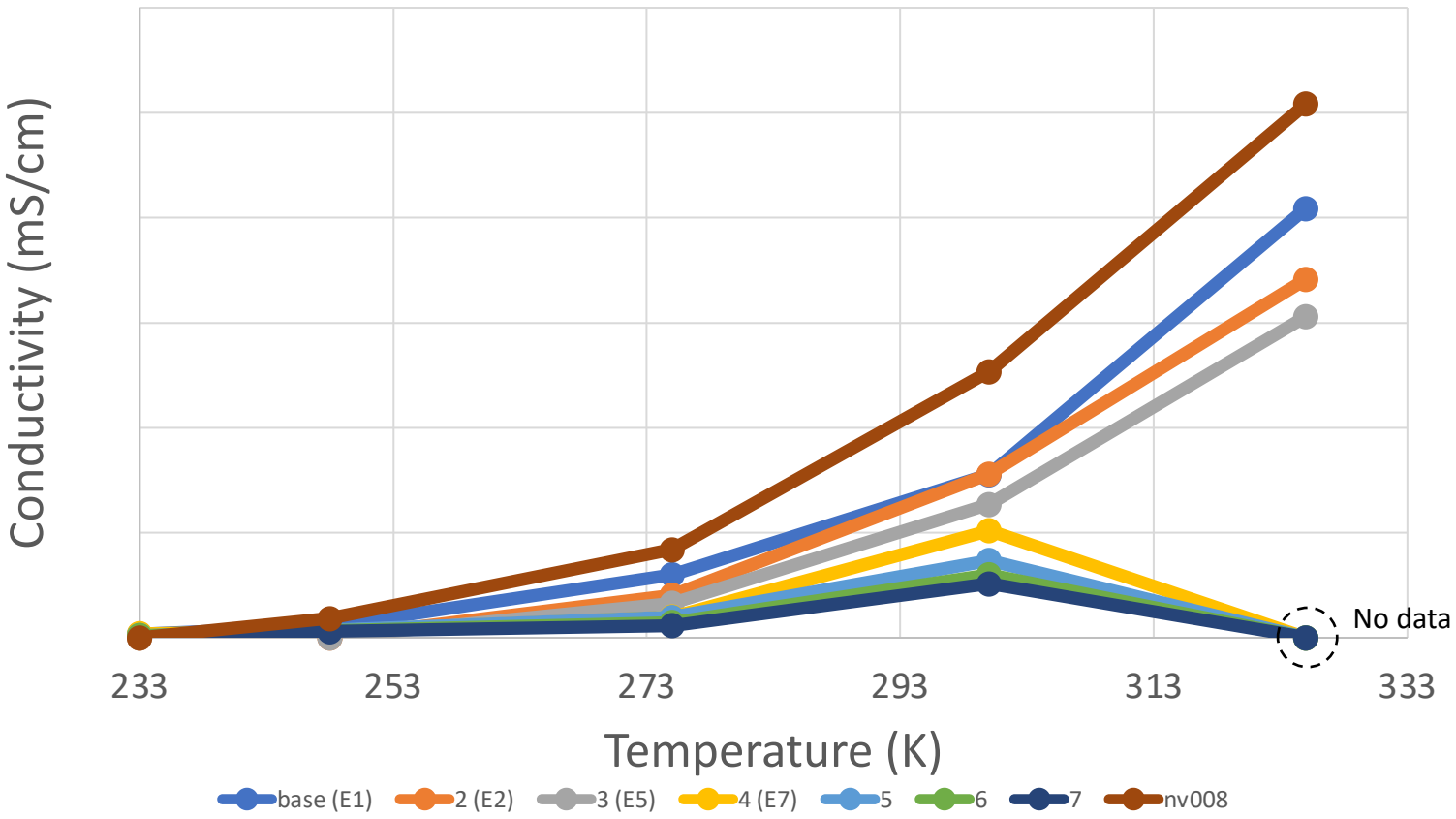





Public

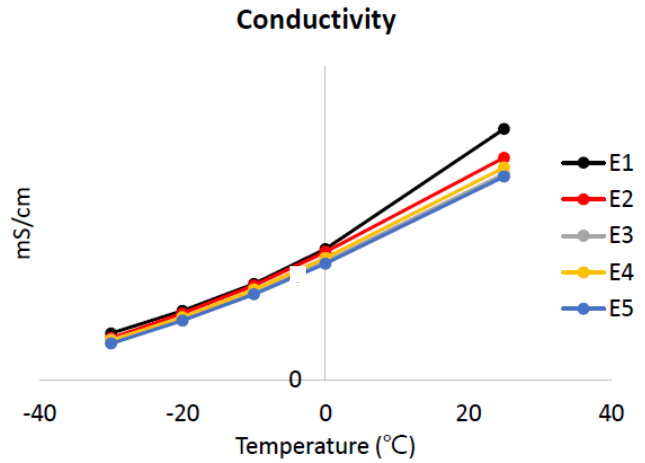
# Electrolyte – Temperature dependence

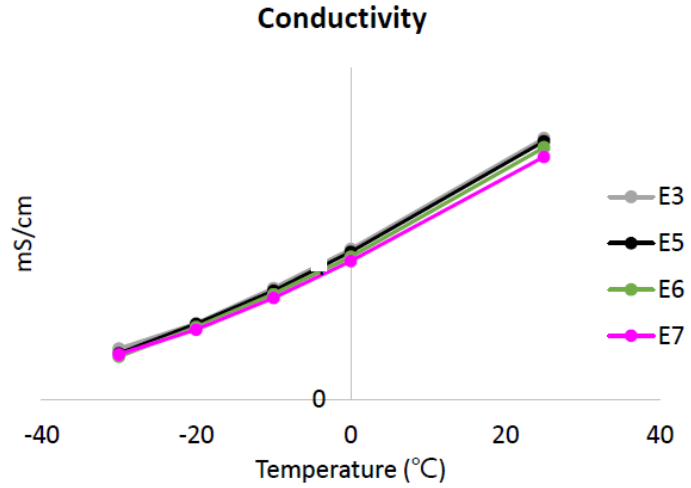
**Computed**




**base (E1) >= 2 (E2) > 3 (E5) > 4 (E7) > 5 > 6 > 7**

**Experimental**




Conductivity:

- E1>E2>E4>E3=E5
- E3=E5>E6>E7

Public

# Research lines - Electrolyte

## Bulk properties

- Ionic conductivity
- Diffusion coefficient
- Dielectric constant
- Chemical stability
- Viscosity
- …

## Local properties

- Solvation structures
- Free solvent percentage
- Solvation shell composition
- Ion-pair lifetime
- Desolvation energy
- …

## Molecular properties

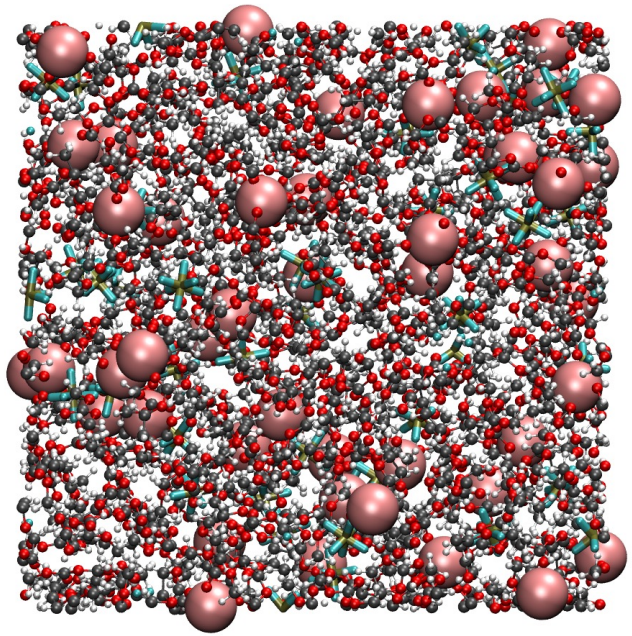
- Energy
- HOMO-LUMO levels
- Charge distribution
- Reaction pthway
- …

© 2021 Northvolt AB, Strictly Confidential

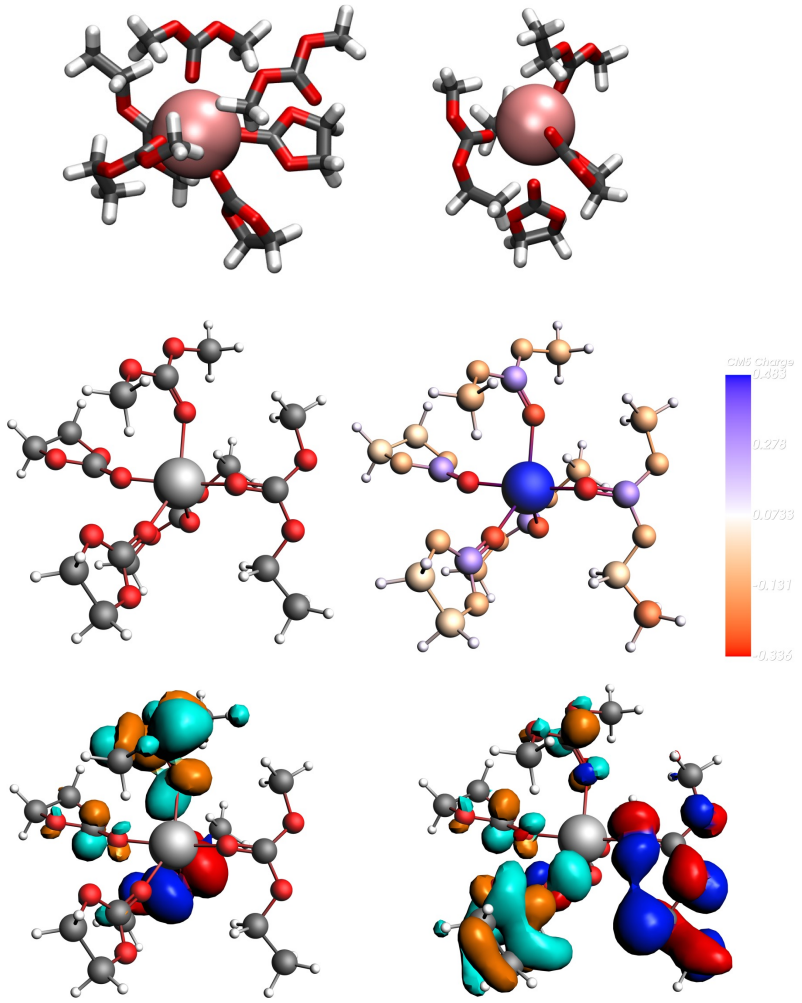
Public

# Research lines - Electrolyte

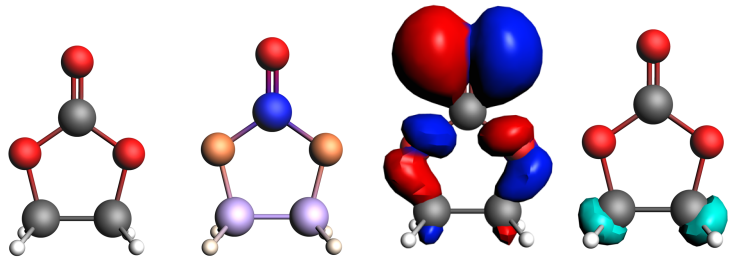
## Bulk properties

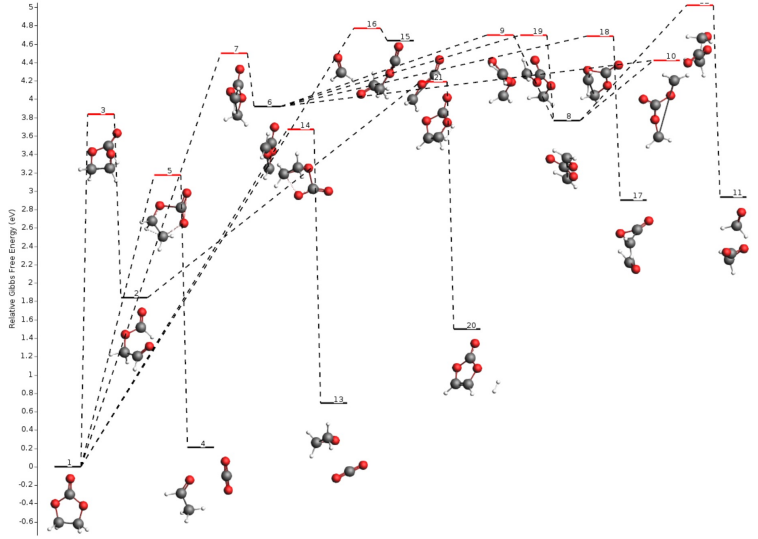


## Local properties




## Molecular properties



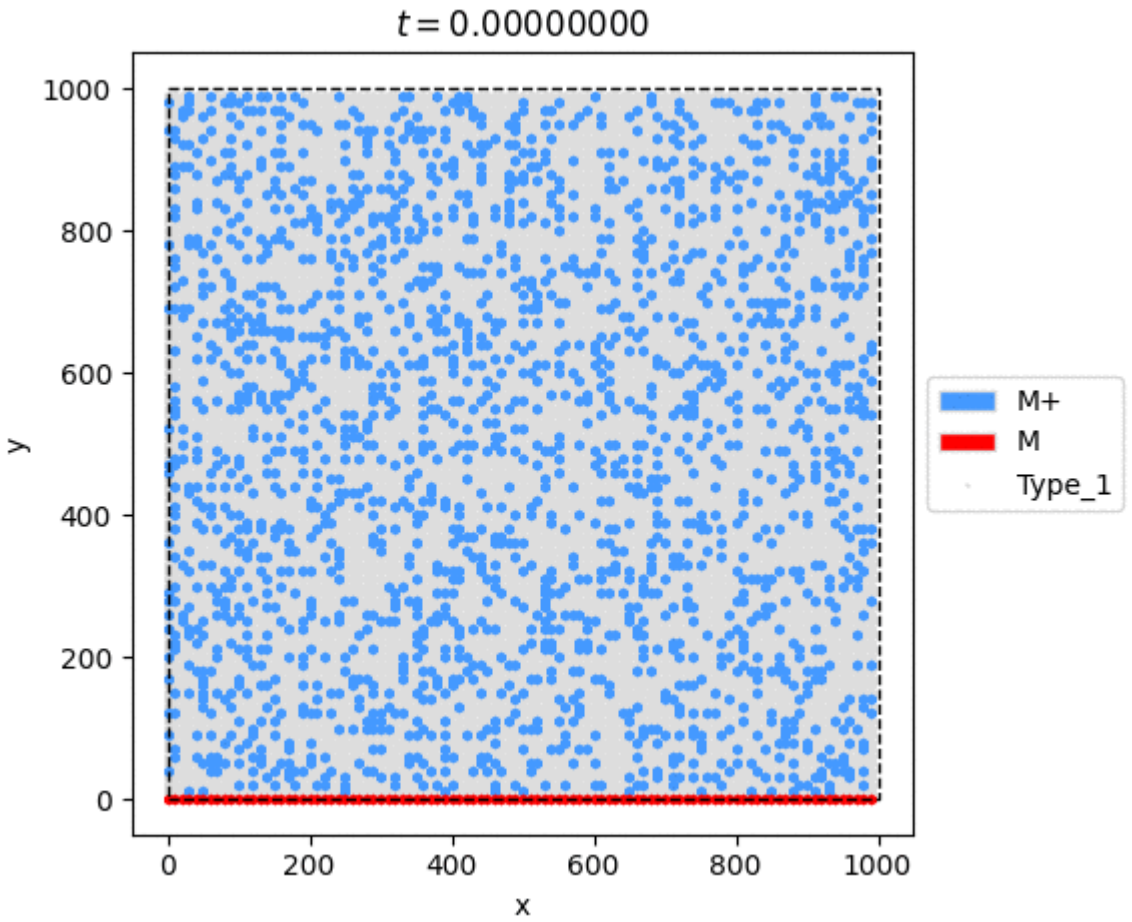



© 2021 Northvolt AB, Strictly Confidential

northvolt

Public

# Dendrites




**M+** : Metallic ion
**M** : Metal atom
**Type_1** : Vacuum spot

**t** : Time (seconds)
**x/y** : Number of sites which correspond to a real length of 0.35 um

There are 3 main reactions happening:

1. **M+** diffusion
2. **M+** → **M** reduction
3. **M** diffusion on the surface


© 2021 Northvolt AB, Strictly Confidential

Confidential

# Acknolegments



Dr. Lilit Axner
Dr. Roberto Di Remigio

northvolt

Public

# Stay in touch

hi@northvolt.com

matteo.ambrosetti@northvolt.com

https://northvolt.com


Public