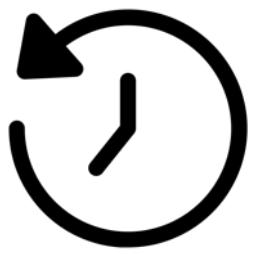


ccmpular

INNOVATIVE ANALYSIS SOFTWARE IMPROVING BATTERY MATERIALS DEVELOPMENT

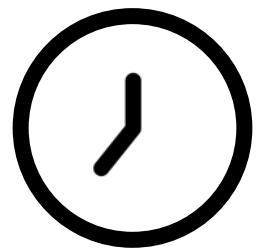
Compular AB
ENCCS Industry Days 2022
October 10, 2022





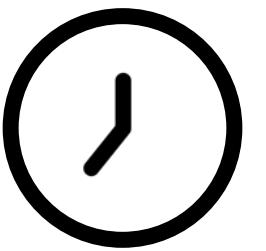
THEN: DRAWING BOARDS





NOW: COMPUTER-AIDED DESIGN (CAD)





NOW: MANUAL LAB WORK





TOMORROW: COMPULAR AIDED DESIGN

The image shows a person's hands interacting with a laptop computer. The laptop screen displays the Compular software interface, specifically the 'Systems' section under 'Species properties'. The interface includes a navigation bar with 'Create new system', 'Systems', 'Composition collection', and 'Settings'. A dropdown menu shows 'System 4'. The main area shows a table titled 'Compare species' for 'Li+' with columns for Number, Structure, Topology, Probability, and Mass. Below this is a table titled 'EC' with columns for Number, Structure, Topology, Probability, and Mass. Both tables contain five rows of data, each with a small molecular structure diagram and numerical values. The laptop is placed on a light-colored wooden surface.

Systems

Species properties

Curve plot

Compular

System overview

System 4

Edit View

Compare species

Li+

Number	Structure	Topology	Probability	Mass
1		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
2		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
3		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
4		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
5		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX

EC	Number	Structure	Topology	Probability	Mass
1	5%		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
2	12%		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
3	10%		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
4	9%		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX
5	5%		$[\text{Li}(\text{TFSI})_2(\text{ACN})_3]^+$	20.8 ±	XXX

TRADITIONAL TRIAL-AND-ERROR R&D LEADS TO LOW PRODUCTIVITY



LONG TIME TO REACH
OPTIMAL COMPOSITIONS



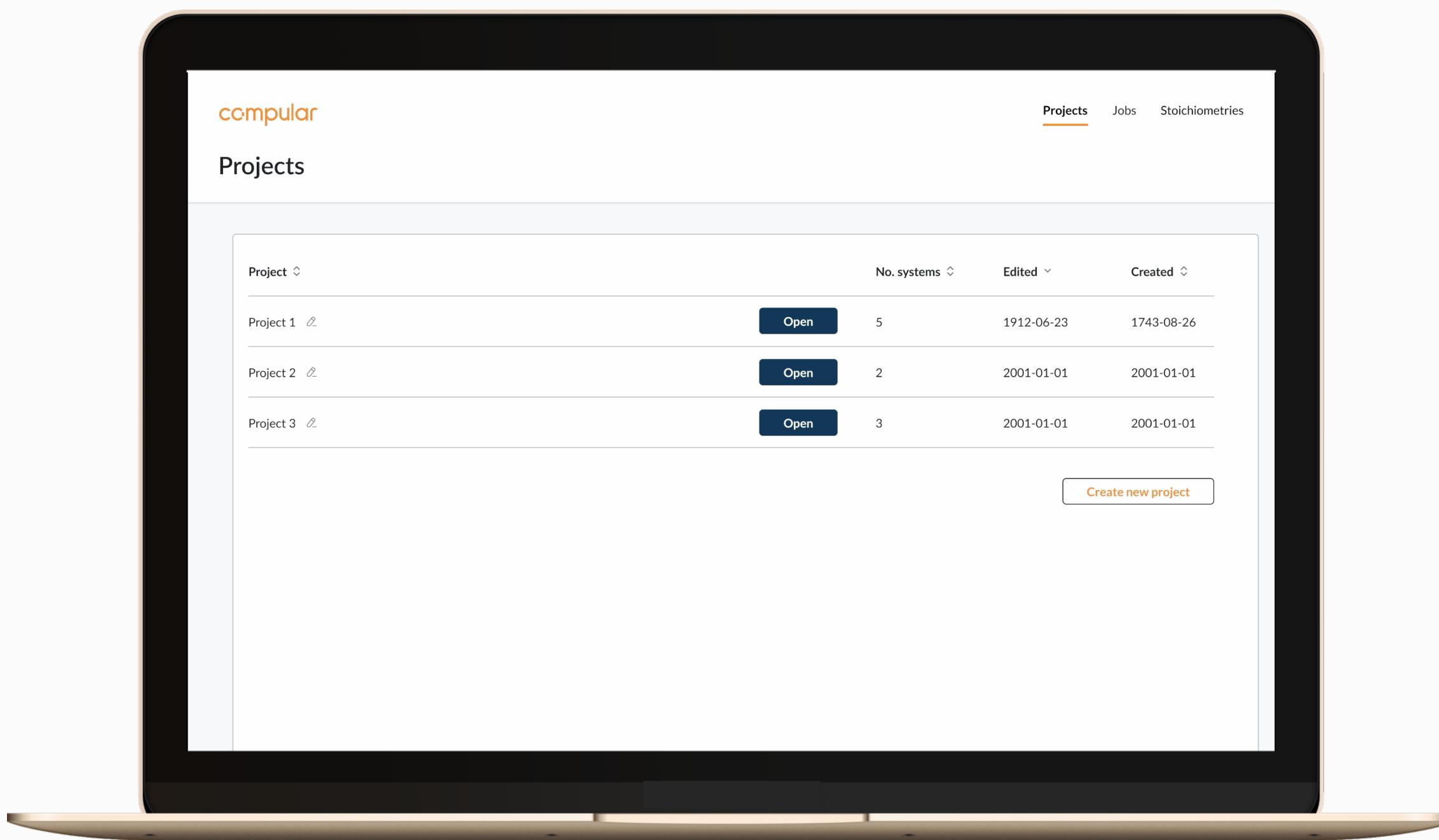
HIGH COSTS IN SALARIES,
EQUIPMENT AND MATERIALS



UNCERTAIN AND
UNRELIABLE PROCESSES



COMPULAR'S DIGITAL MODELLING IS THE NEW BLACK



DIGITAL SCREENING OF CHEMICAL
SYSTEMS THROUGH SIMULATIONS



RELEVANT PERFORMANCE
PROPERTIES AS OUTPUT

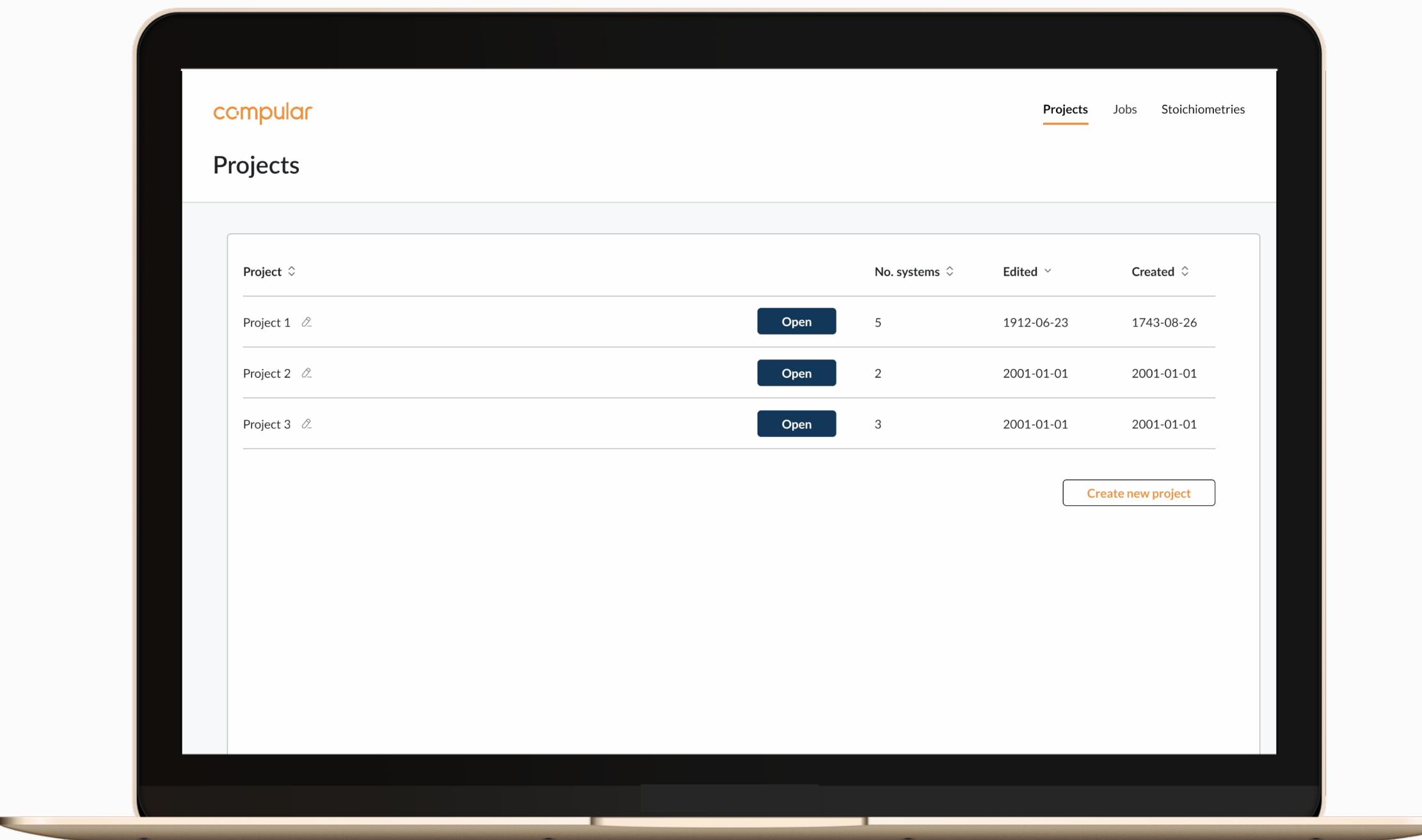


QUICK, RELIABLE
AND EASY TO USE



FROM YEARS OF WORLD-LEADING
RESEARCH AT CHALMERS UNIVERSITY

COMPULAR'S DIGITAL MODELLING IS THE NEW BLACK

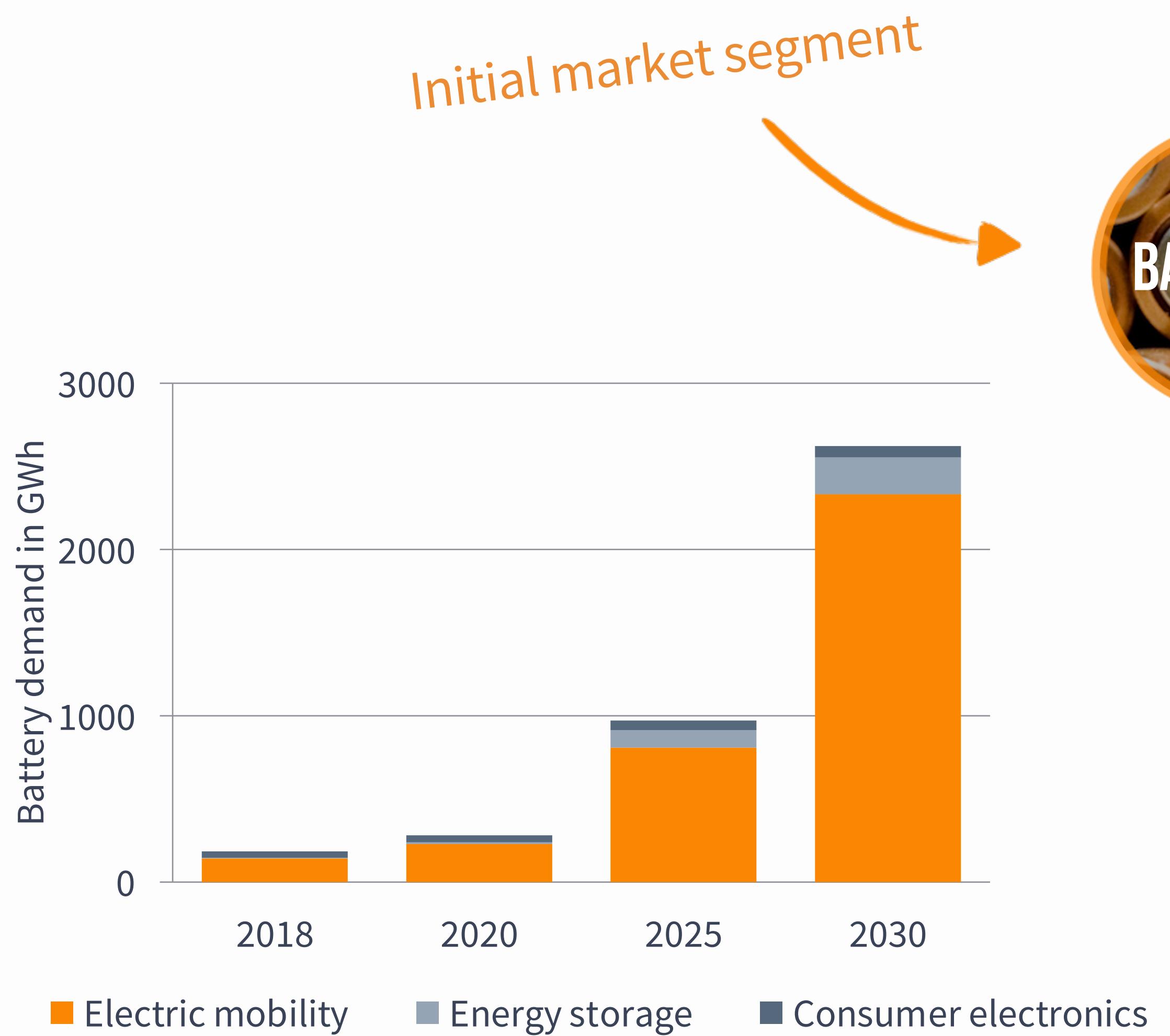


Higher lab trial **success rates**

Faster product development cycle

Enabling more **qualitative & innovative products**

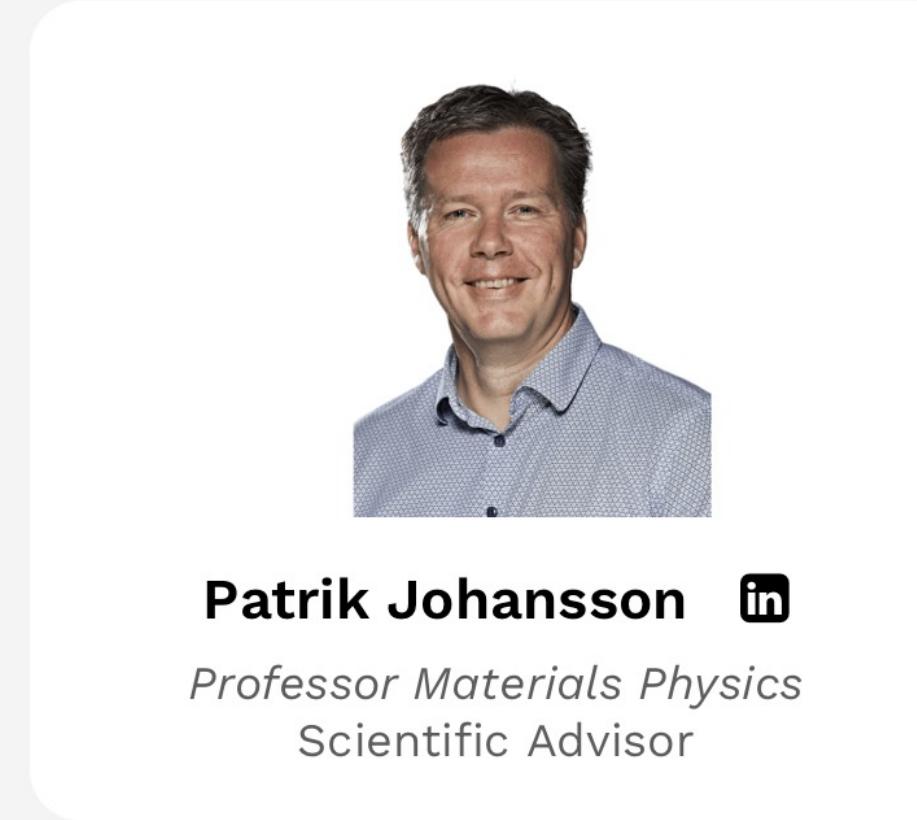
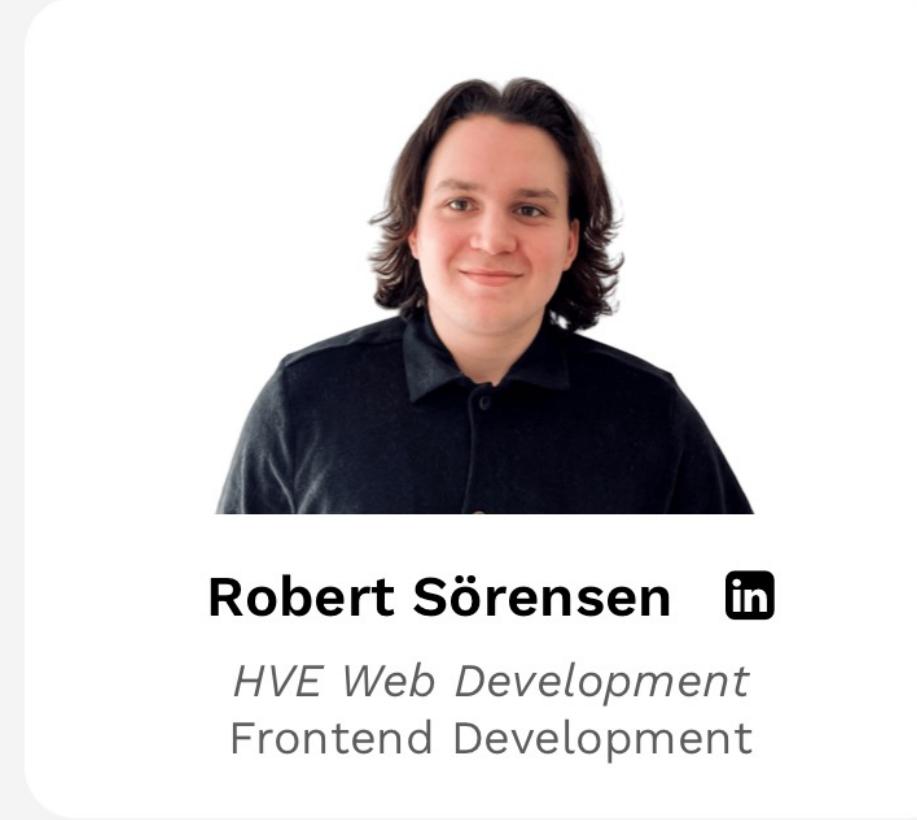
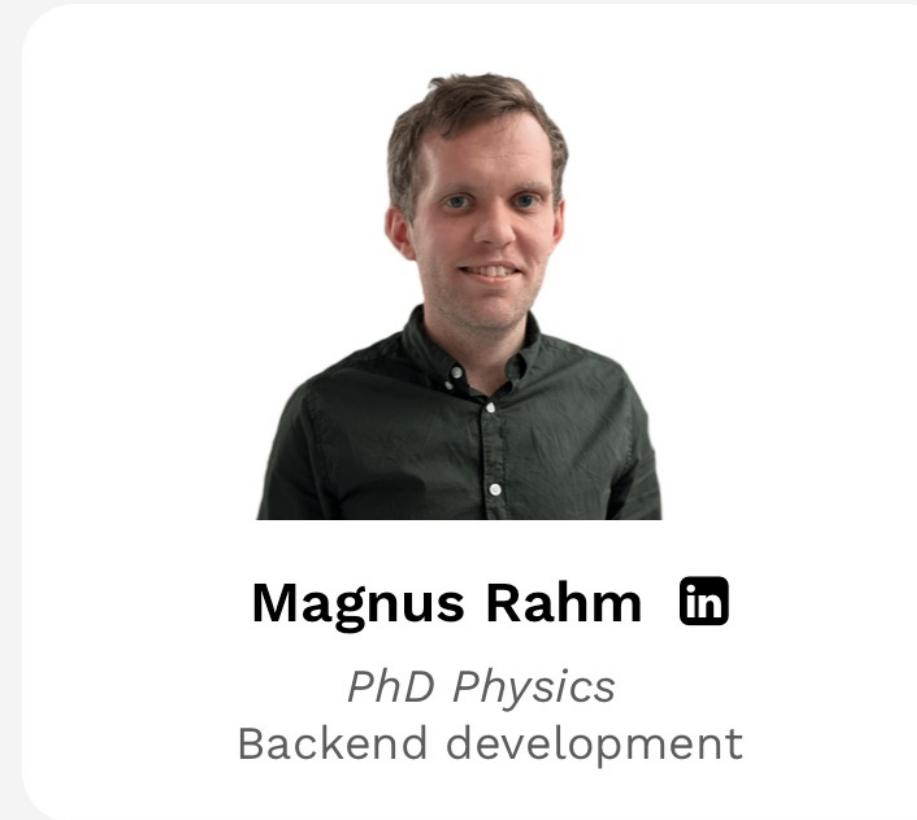
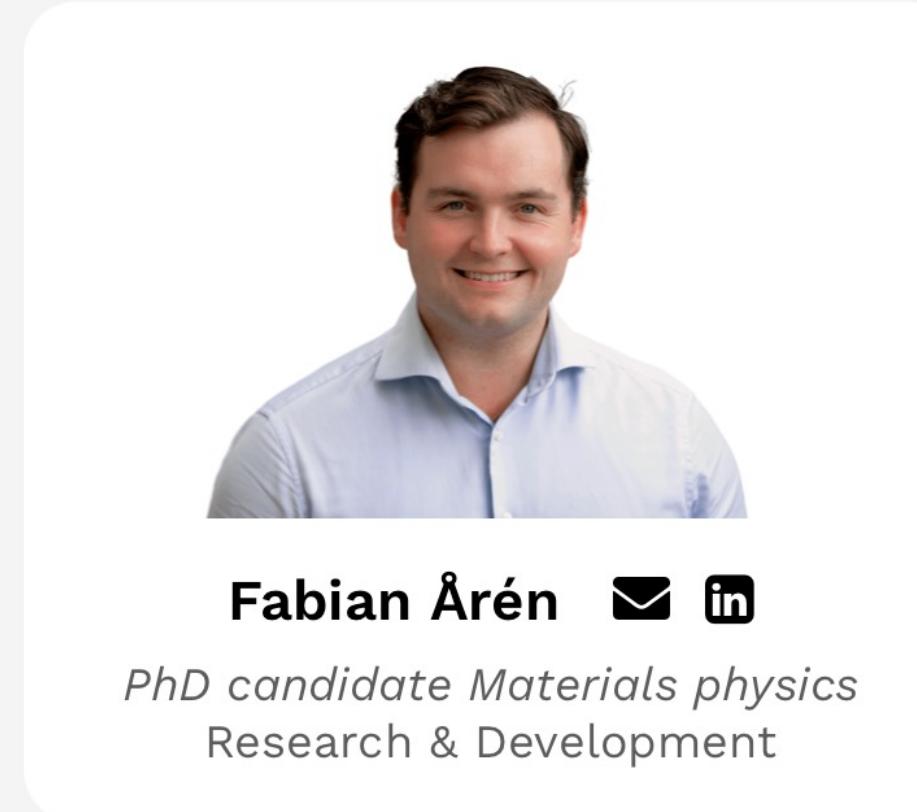
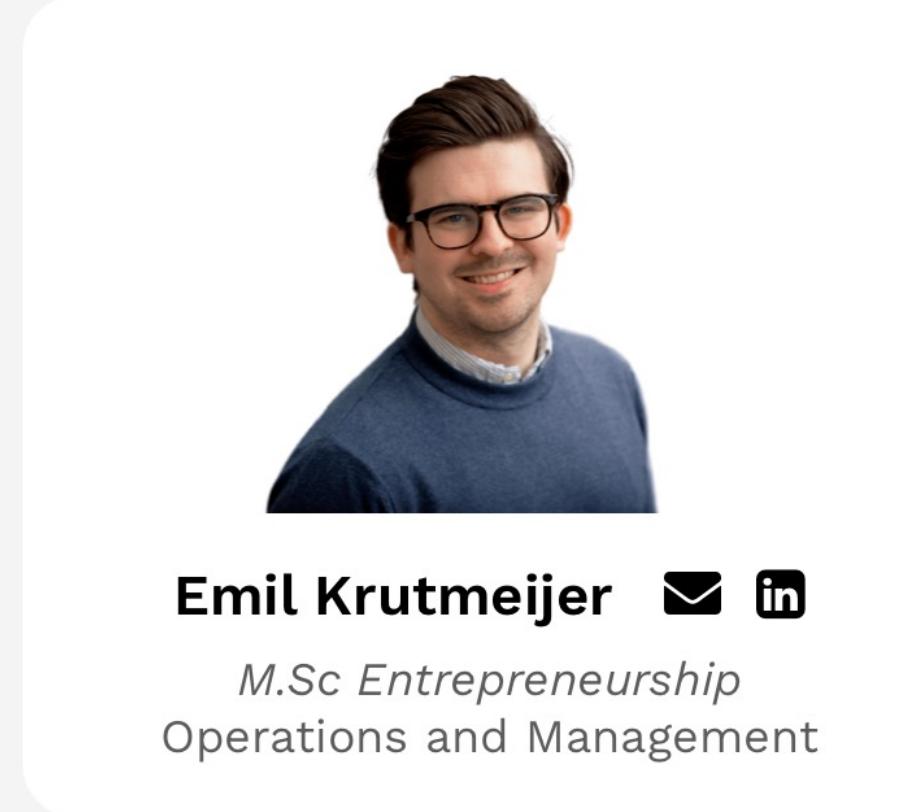
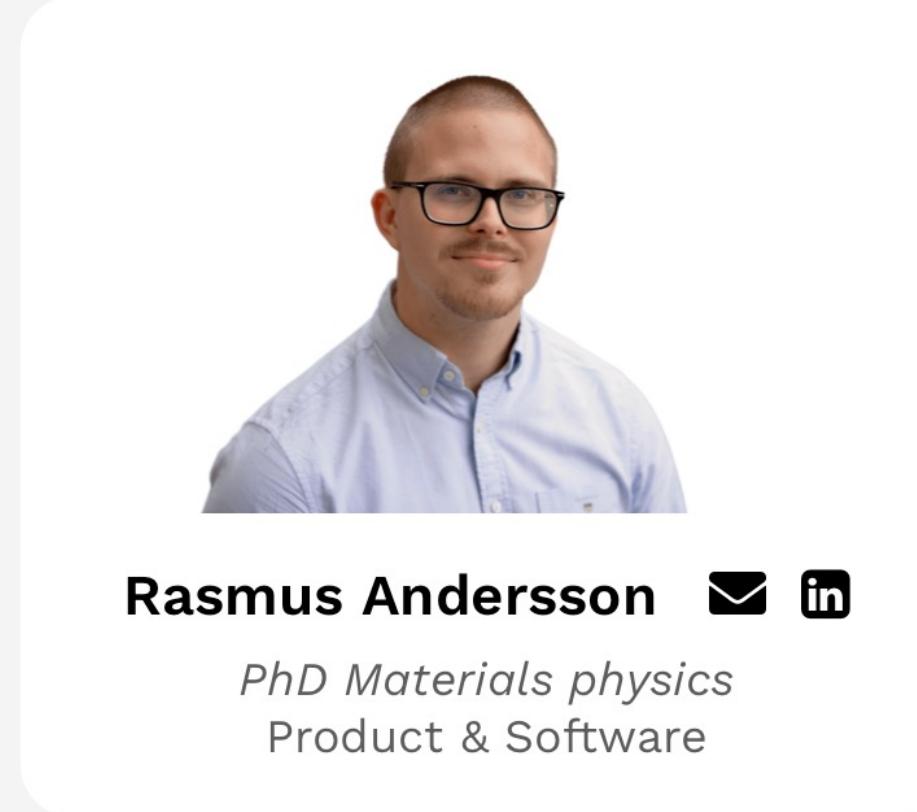
MARKET SEGMENTS



Source: World Economic Forum: McKinsey, 2020

© Compular 2021

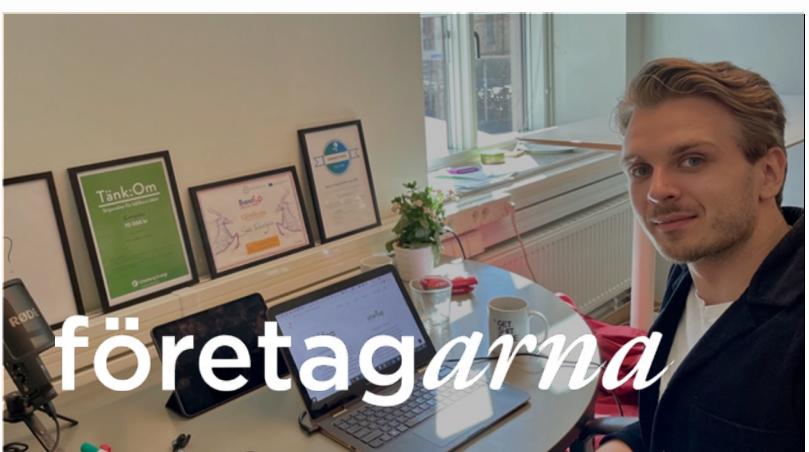
TEAM



Bragging



StageTwo: Best European university-tech spinout



Top 103 entrepreneurs under 35 years



EIT Manufacturing
BoostUp North winner

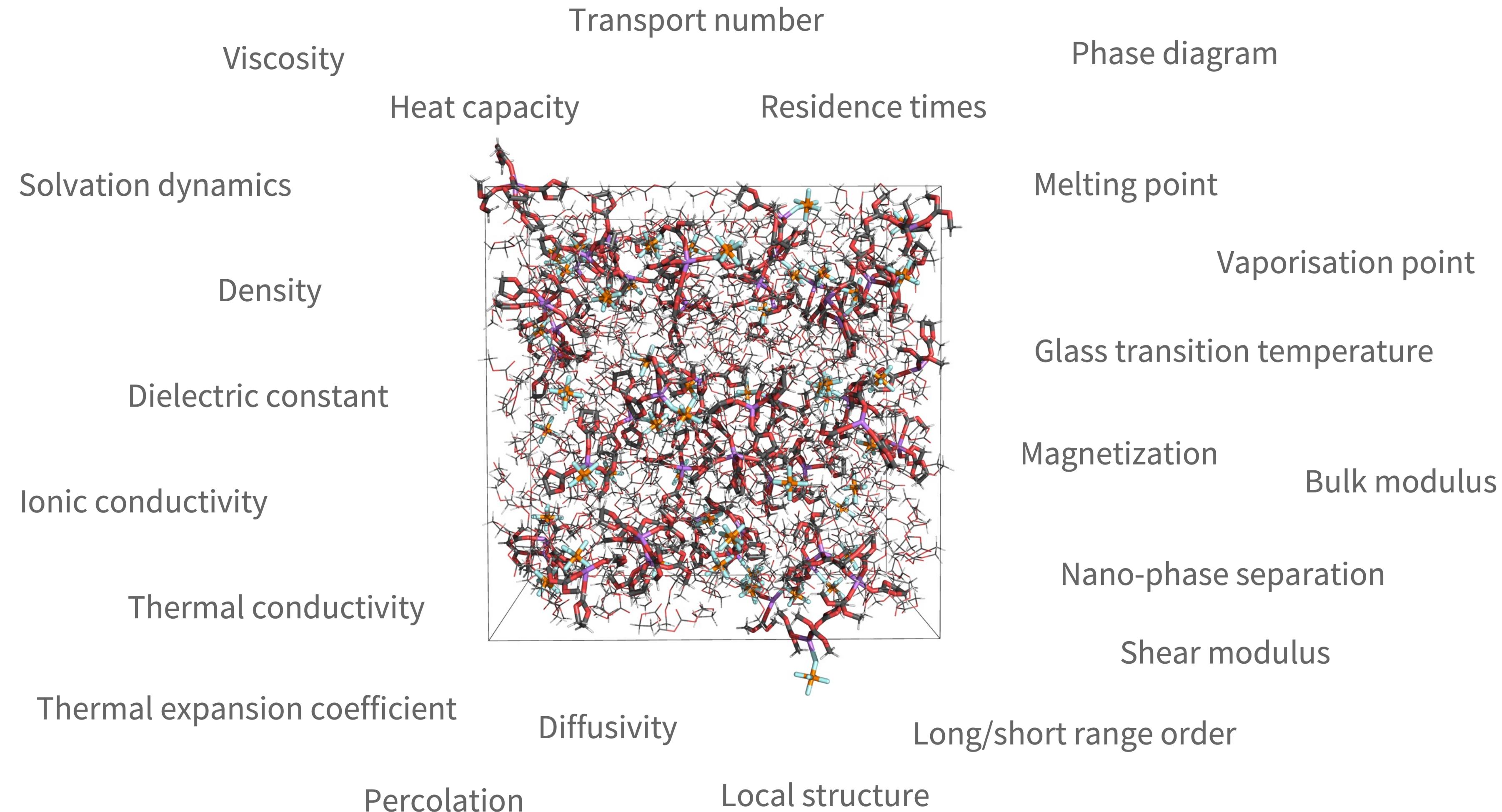


County winners of SKAPA-Talang for young innovators



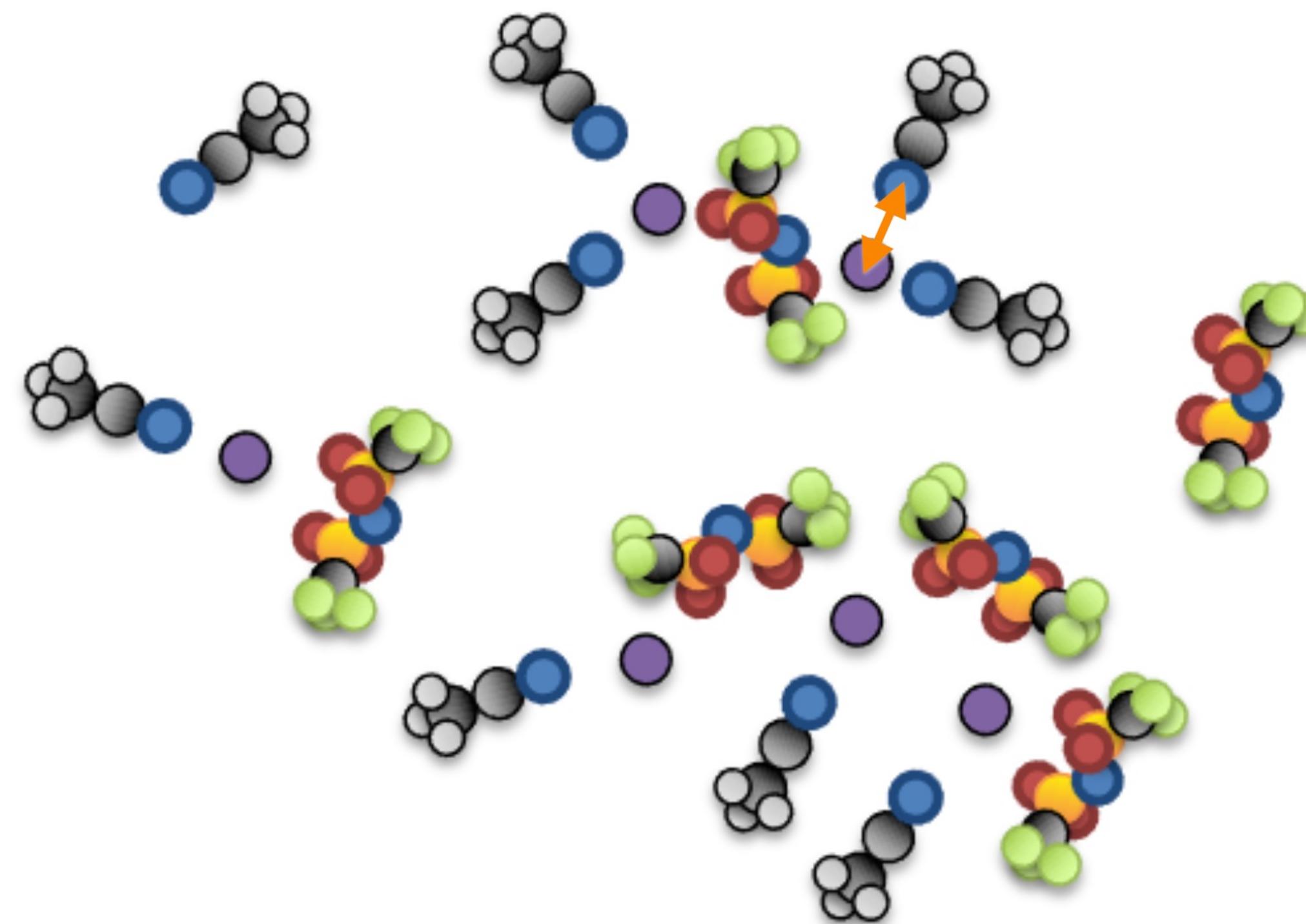
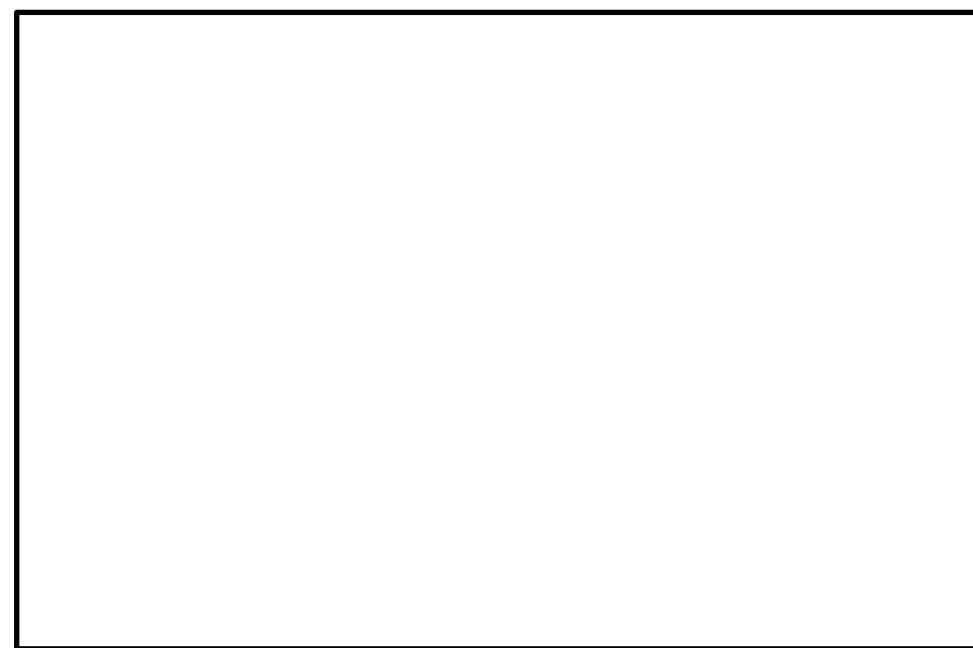
Venture Cup winners - beyond academic

Method Background

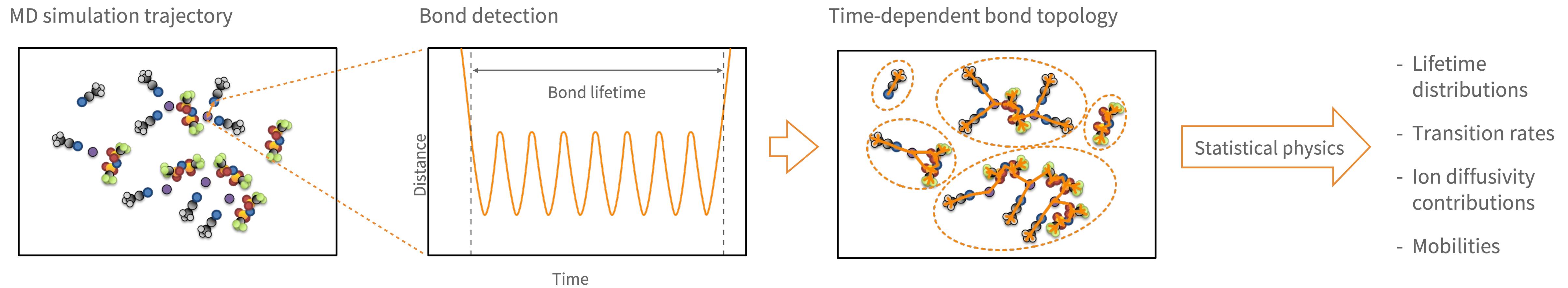


Method Background

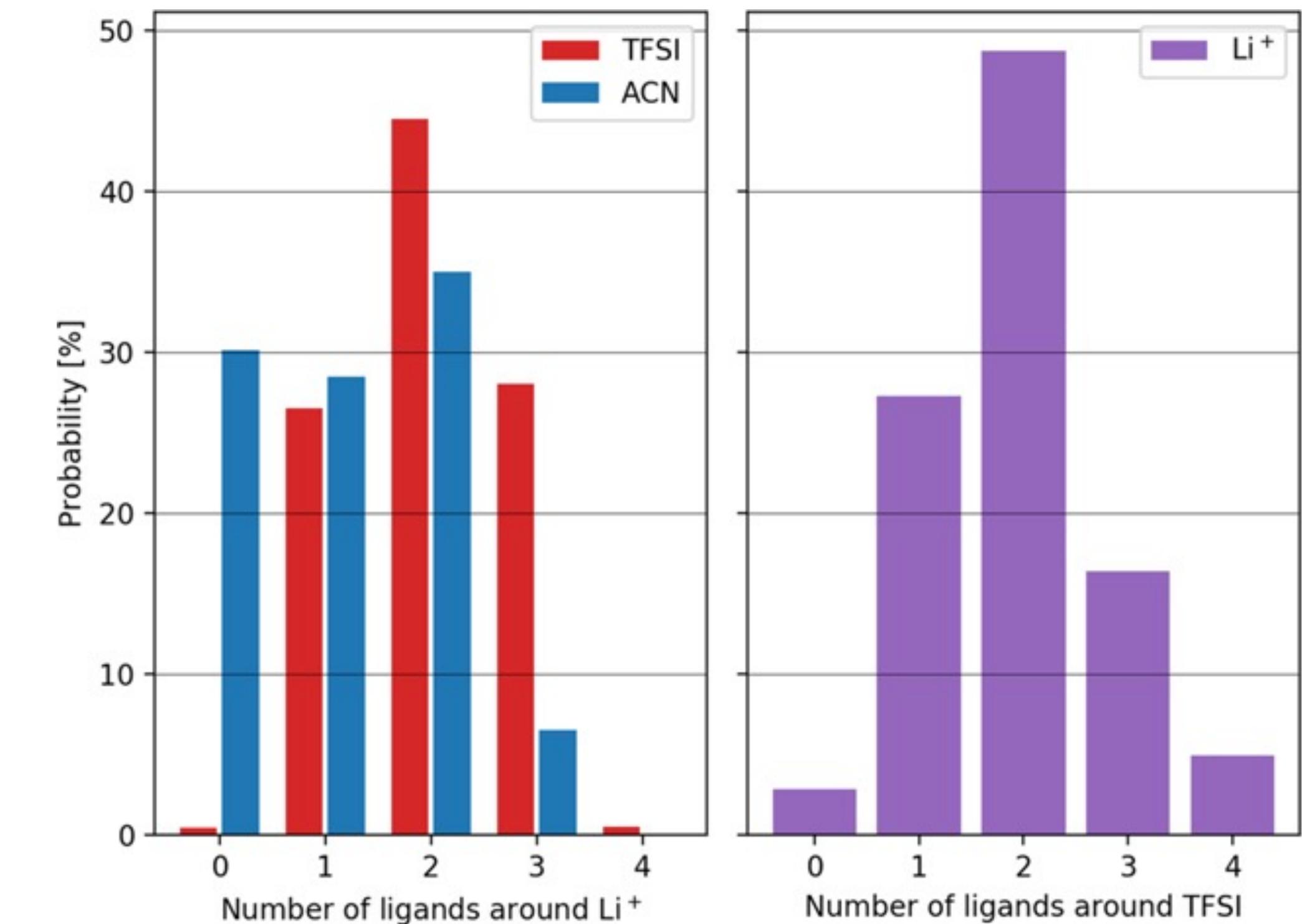
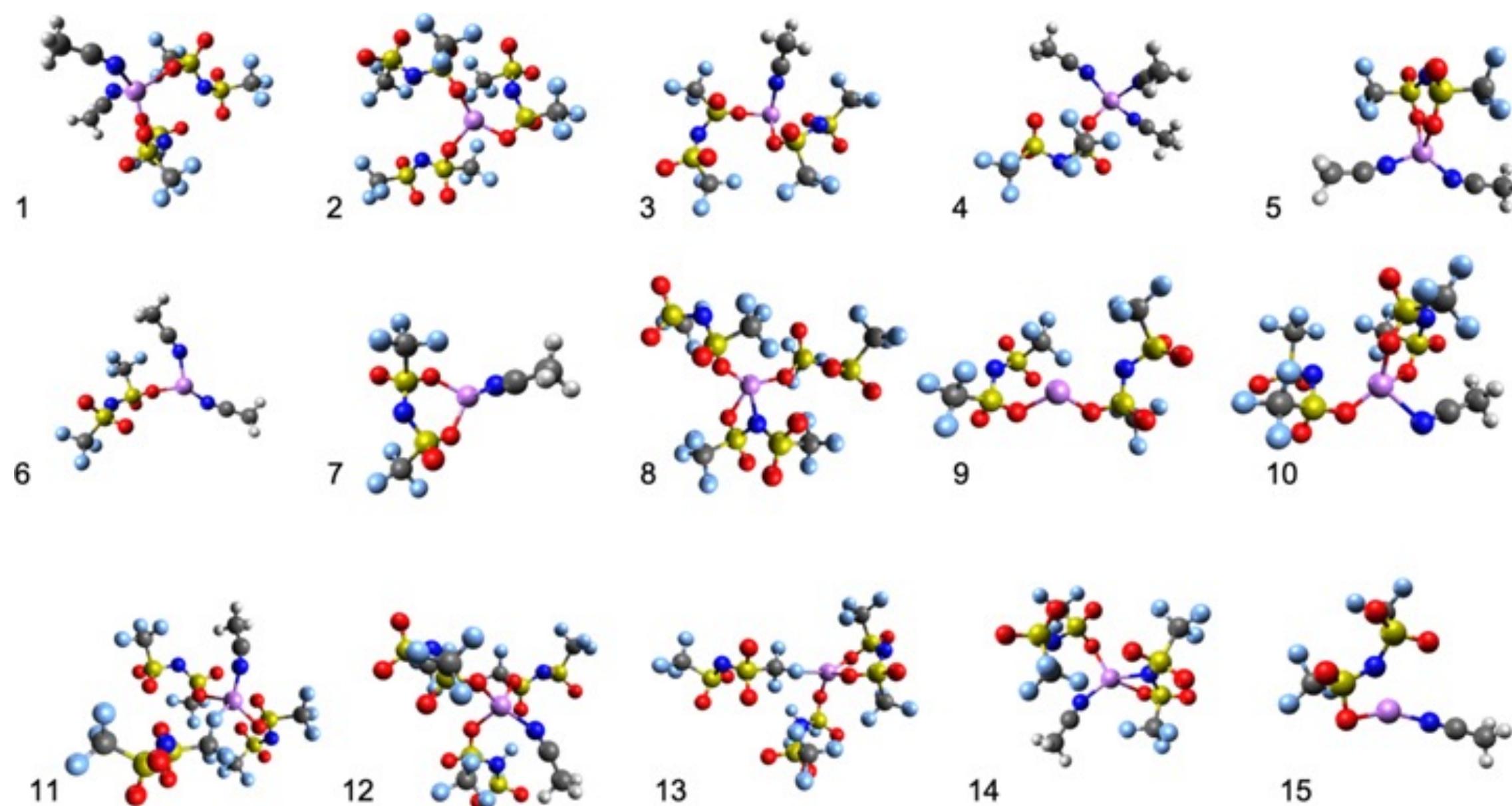
MD simulation trajectory



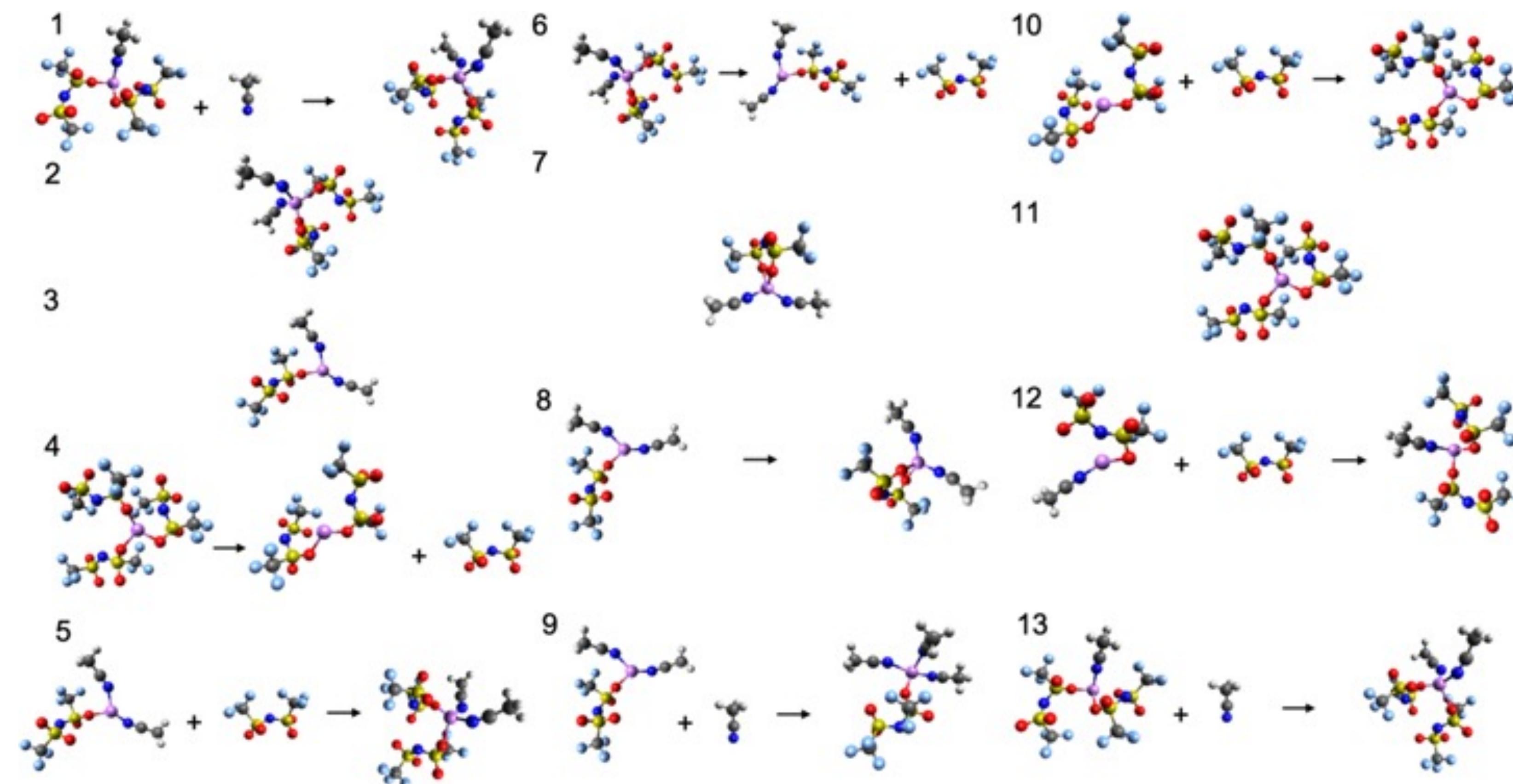
Method Background



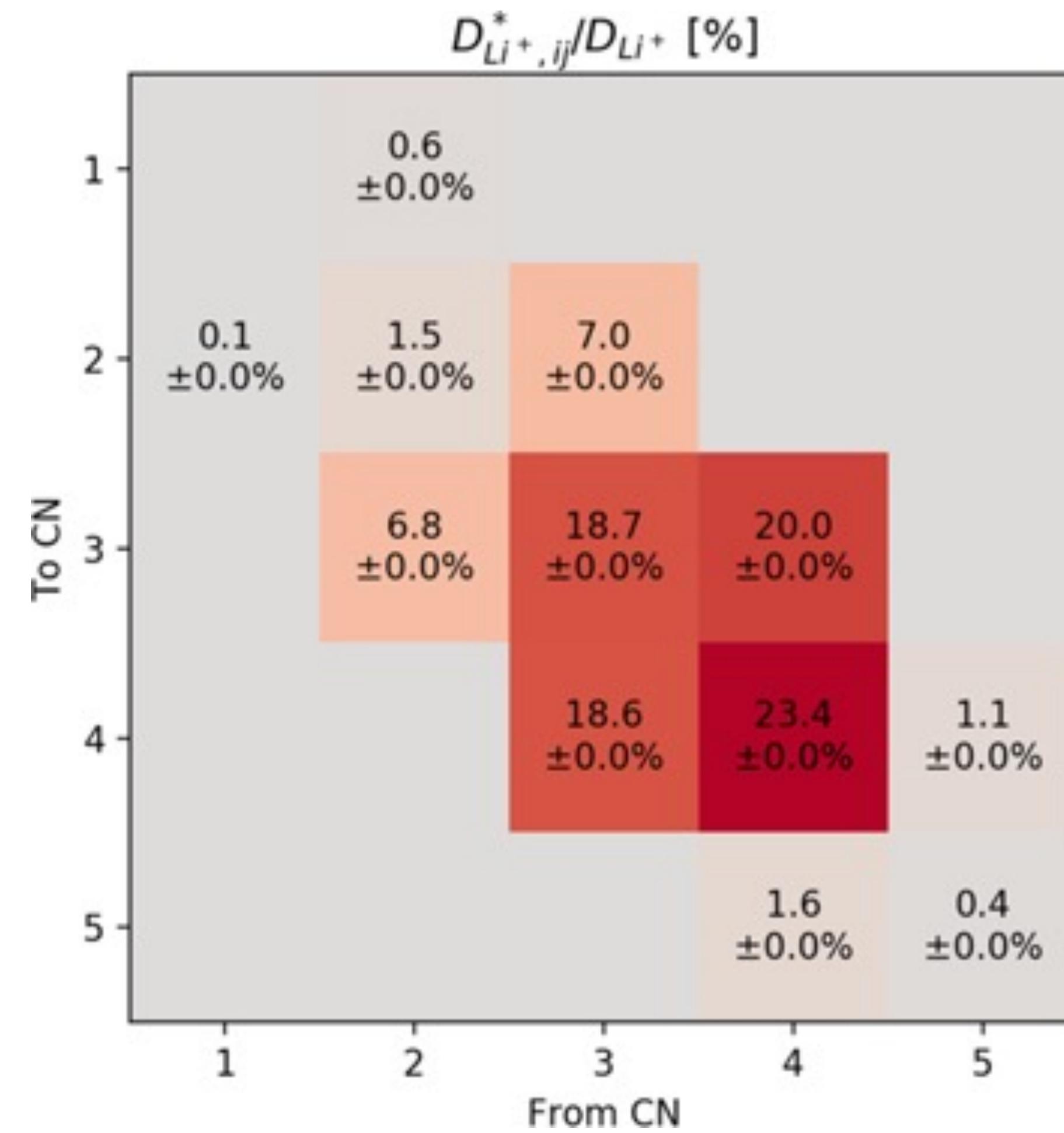
Method Background



Method Background



Method Background



Method Background

Summary

- Unique method enabling bond graph topology detection
- Procure both experimentally comparable results and deeper understandings
- Cut down on labour intensive manual work in favour of computational methods



FF4EuroHPC Call2

Overview

- FF4EuroHPC Call 2
- **Molecular Dynamics** Simulations and Analysis for Improved **Battery** Materials **Development** (MDBD)
- March 2022 – March 2023
- Showcase the advantages and possibilities that computational modelling brings to the battery space



FF4EuroHPC Call2

Consortium

ccmpular



FF4EuroHPC Call2



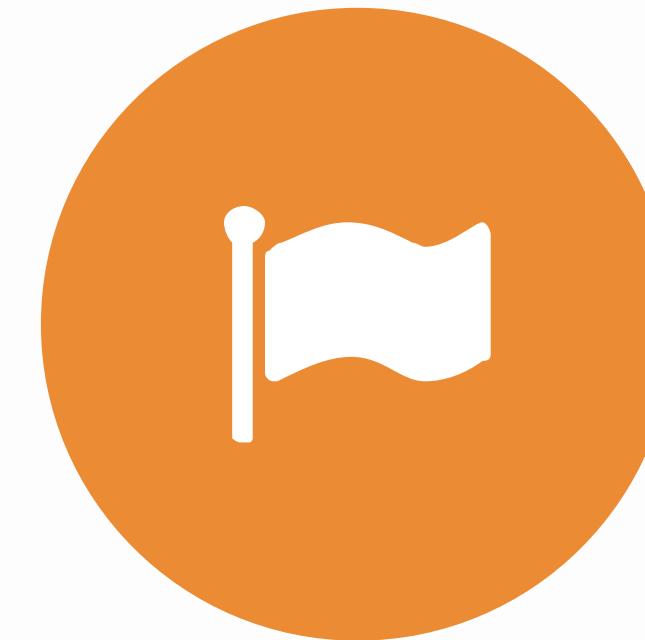
Why?

Enabling better
battery solutions for a
more sustainable
future



How?

Simulating and
analysing properties of
importance for battery
developers



What?

Showcasing the
advantages of using
digital modelling and
HPC-resources

FF4EuroHPC Call2

Progress

-  Detailed work plan and specification of suitable compounds and analysis routines
-  Creation of simulation and analysis routines
-  Setting up infrastructure and processes on HPC-system Karolina
-  Gaining preliminary results for a time step selection and time to structural equilibration
-  Production runs (variables: density, temperature, pressure)
-  Prediction of e.g. density, ionic conductivity, viscosity and salvation structures
-  Experimental validation of predictions



*Digitalising material development:
for a more sustainable future.*

compulartech.com

info@compulartech.com

+46(0)70 685 17 17 (Emil)

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References

- **Proof of concept of method/software**
R. Andersson, F. Årén, A. A. Franco and P. Johansson, Ion Transport Mechanisms via Time-dependent Local Structure and Dynamics in Highly Concentrated Electrolytes, *Journal of the Electrochemical Society*, 2020, DOI:10.1149/1945-7111/abc657
- **Application to hybrid HCEs**
P. Jankowski, R. Andersson and P. Johansson, Designing high-performant lithium battery electrolytes by utilizing two natures of Li⁺ coordination: LiTDI/LiTFSI in Tetraglyme, *Batteries & Supercaps*, 2020, 4(1), 205-213, DOI:10.1002/batt.202000189.
- **Application to LP30**
R. Andersson, O. Borodin, and P. Johansson. "Dynamic Structure Discovery Applied to the Ion Transport in the Ubiquitous Lithium-ion Battery Electrolyte LP30." *Journal of The Electrochemical Society* (2022).
- **Doctoral dissertation**
R. Andersson, Dynamic Structure Discovery and Ion Transport in Liquid Battery Electrolytes, Chalmers University of Technology, 2020
- **Method description**
R. Andersson, F. Årén, A. A. Franco and P. Johansson, CHAMPION: Chalmers Hierarchical Atomic, Molecular, Polymeric & Ionic Analysis Toolkit, *Journal of Computational Chemistry*, 2021, DOI:10.1002/jcc.26699