

# Molecular Dynamics Simulations for New Battery Materials Development

## Organizations

**Enerpoly** is an energy storage technology SME pioneering the rechargeable zinc-ion battery chemistry.

**Compular** is an SME developing HPC software for simulating and analysing molecular dynamics in material development projects.

**Chalmers Industriteknik** is a non-profit foundation offering academic expertise within the areas of materials, energy, and digitalization.

**ENCCS** is an initiative aiming to provide a unified HPC know-how hub for academia, industry, and the public sector.



End User



ISV



Technology Expert



HPC Expert

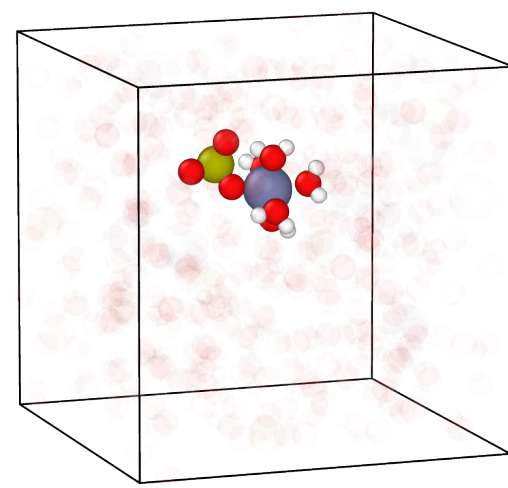
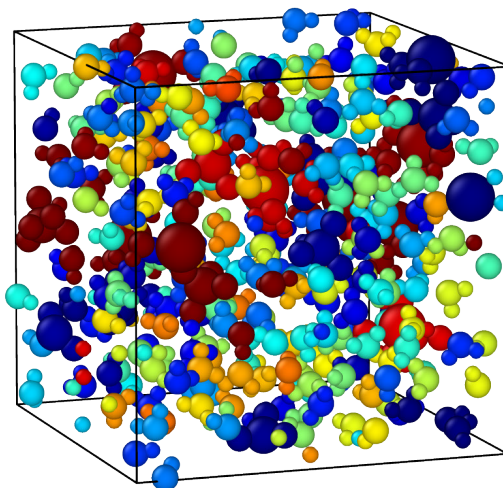
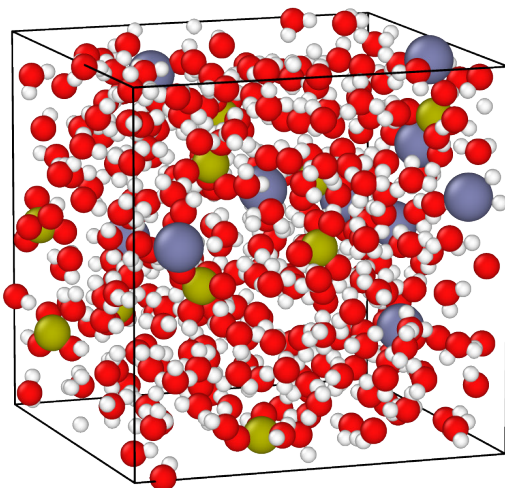


ENCCS is part of the Swedish NCC.



## The Challenge

Enerpoly, developing new battery solutions based on zinc-ion technology, faces serious problems such as irreversible loss of charge or material. To better understand the relevant properties of electrolytes without expensive and time-consuming lab tests, Enerpoly would like to use Compular's in-house simulation tool based on a novel and patent-pending combination of molecular dynamics (MD) simulations and trajectory analysis of charged particles, not yet available as a product.





Industry Sector  
**Energy**

Technology used:  
**HPC,  
AI,  
Molecular Dynamics  
Simulations**

## The Solution

The experiment tackled both technical and business challenges by transforming Compular's existing command-line-driven software stack into a product called CHAMPION, marketed on a pay-per-use basis and giving customers like Enerpoly an easy way to solve their problems.

CHAMPION analyses the results of external MD simulations running on HPC to determine bonds in particle trajectories and detect molecular structures in the electrolyte relevant to battery chemistry performance. CHAMPION now provides a user-friendly solution by managing the coupling with an open-source MD code running on an HPC infrastructure as it requires about 1,000-10,000 core hours per simulation.

This workflow was validated on Enerpolys' existing zinc-ion battery system at different temperatures and pressures, ensuring that it gives correct results and is trustworthy for future use on unknown, novel material combinations and battery systems, thus demonstrating the ability to predict material properties of different chemical compositions.

## The Impact

As the first user of Compular's newly developed in-silico framework for materials properties prediction, Enerpoly now has the tools to cut down battery material R&D time and lab testing costs significantly. By running the MD simulations themselves, they better understand how different compositions and conditions lead to desired material properties. Thus, Enerpoly is able to shorten time-to-market for novel, better-performing and more affordable batteries, which is essential for the company's competitiveness in this fast-moving field.

Compular's potentially game-changing technology was transformed into a software product, CHAMPION, sold through a new competitive SaaS pay-per-HPC-analysis business model. This opens new market opportunities in the dynamic battery sector, with the potential to expand to other markets (e.g. composites) in the next 3-5 years. Furthermore, this experiment and growing interest from the battery industry has already secured 3 new paying customers with the full European market launch expected in 2023. Consequently, the company grew from 3 to 7 employees with further hires anticipated in 2023.

## Benefits

- Enerpoly can run millions of experiments in silico compared to 10 experiments per month in a lab.
- Enerpoly reduced lab experiments by 20% and related costs by 20-30% resulting in a 5x- 10x return on investment.
- Estimated 20-40% faster time-to-market for Enerpoly batteries.
- New SaaS business model: Compular already gained 3 new customers and hired 4 new employees.