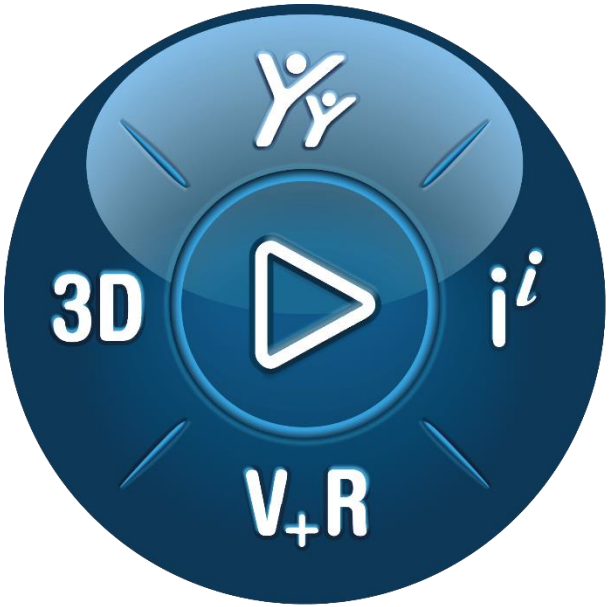


3DEXPERIENCE®

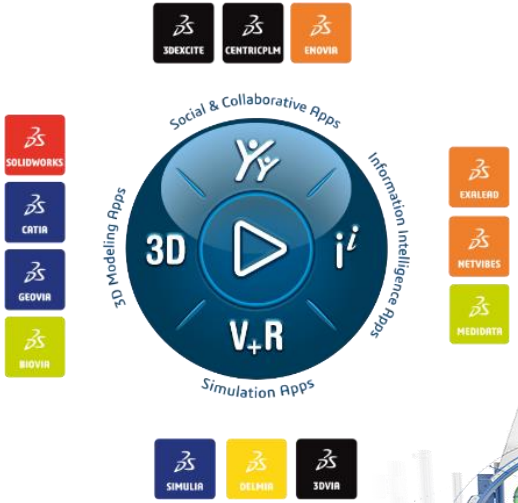
BIG-MAP - Expectations from a Software Developer

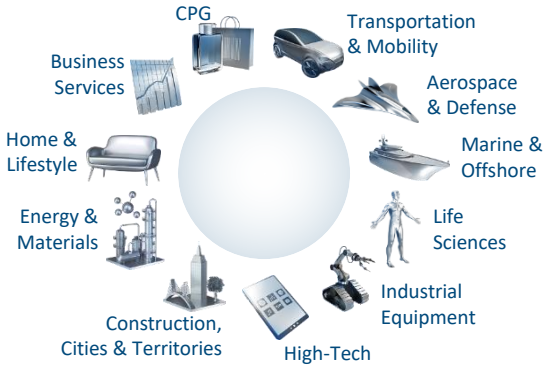
Enabling the Industrialization of Sustainable Batteries

Dr. Johan M. Carlsson
Senior Industry Process Scientist
Fellow BIOVIA Science Council

DASSAULT SYSTEMES | The 3DEXPERIENCE® Company

Dassault Systèmes





1981
3D Design

1989
3D DMU Digital Mock-up

1999
3D PLM Product Lifecycle Management

3DEXPERIENCE®

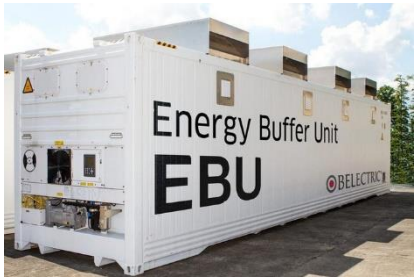
2012
3DEXPERIENCE® platform

2020
Virtual Twin Experience of **Humans**

DASSAULT SYSTEMES

Why is 3DS interested in Batteries?

- New batteries require new materials
  - Handheld electronics and computers
  - Stationary Energy Storage
  - Cars
- Paradigm shift for mobility
  - Biggest challenge is not the power train
  - The challenge is energy storage: Batteries
- 3DS intend to establish a digital twin of batteries and electro vehicles



http://www.apricom-group.com

DASSAULT SYSTEMES

Total Coverage From Chemistry To Systems

Molecular | Cell | Module & Pack | Device

Behavior Models for System Design, Verification & Validation

1D

Aging

Thermal

Electrical
El.-Chem.

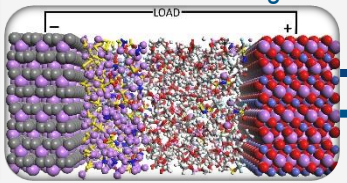
Battery Management System

3D. DESIGN | ENGINEERING | PHYSICS

High-Resolution Models for Detailed Design & Analysis

3D

Molecular level material and chemical modeling



Mechanical | Thermal | Diffusion | Electrical

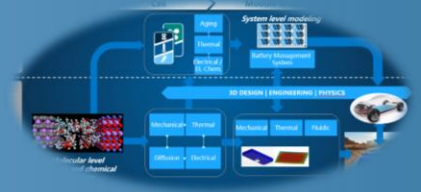
Mechanical | Thermal | Fluid

DASSAULT SYSTEMES

3DEXPERIENCE Platform enables the Industrialization of Sustainable Batteries

ONE 3DEXPERIENCE® PLATFORM FOR

Battery Development from Materials to Systems



Battery Manufacturing Operations

Battery Factory Infrastructure Engineering & Construction

to create the **Virtual Twin Experience** of

Batteries,
from Atoms to Systems

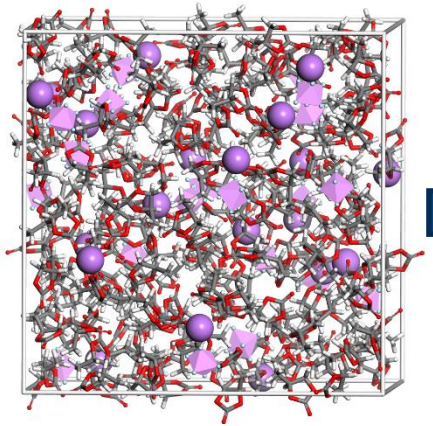
Manufacturing Operations,
including product, process and resources

Gigafactories Projects,
across the lifecycle of the plant

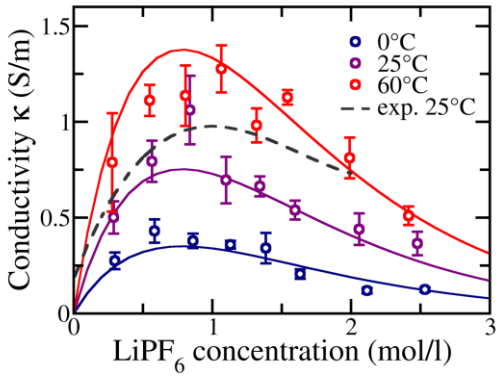
Influence of Electrolyte Performance

Quantitative prediction from Atoms to Cell

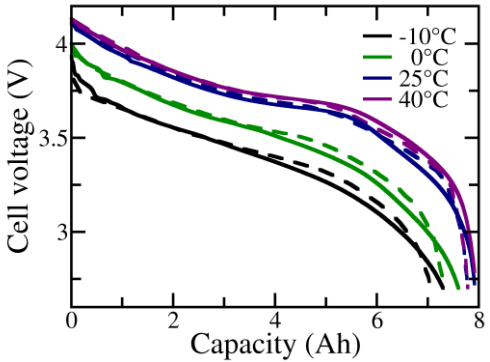
- Solution: in-silico testing of electrolyte formulations from atom to cell



Atomistic model



in-silico engineering characterization



Cell voltage response (measured vs predicted)

- Quantitative cell discharge curves incl. low temperatures and fast discharge

Journal of The Electrochemical Society, 2020 **167** 013522

Multi-Scale Electrolyte Transport Simulations for Lithium Ion Batteries

Felix Hanke,[1,z] Nils Modrow,[2] Reinier L. C. Akkermans,[1] Ivan Korotkin,[3,4] Felix C. Mocanu,[5] Verena A. Neufeld,[5] and Max Veit[6,a]

[1]Dassault Systèmes, CB4 0WN Cambridge, United Kingdom
[2]Dassault Systèmes, IDEON Gateway, 22363 Lund, Sweden
[3]Mathematical Sciences, University of Southampton, SO17 1BJ, United Kingdom
[4]The Faraday Institution, Harwell Campus, Didcot, OX11 0RA, United Kingdom
[5]Department of Chemistry, University of Cambridge, CB2 1EW, United Kingdom
[6]Department of Engineering, University of Cambridge, CB2 1PZ, United Kingdom

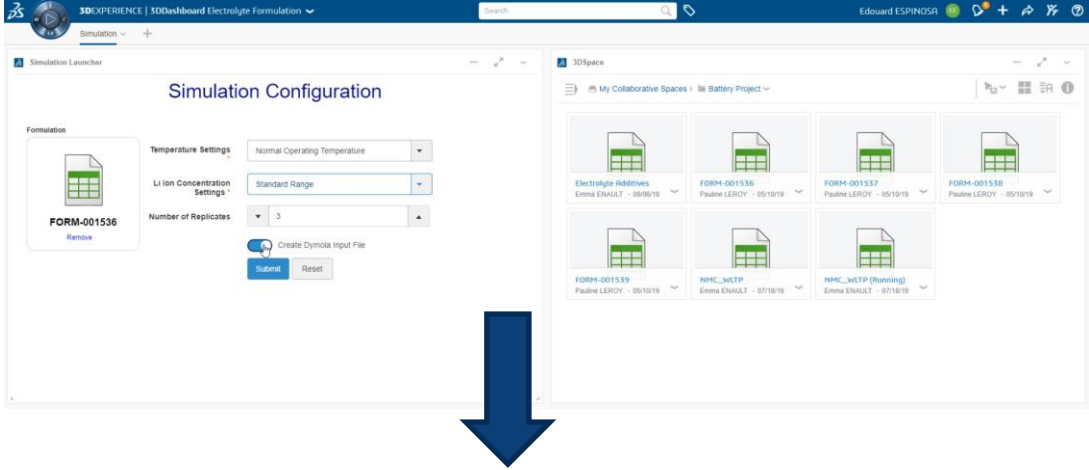
Establishing a link between atomistic processes and battery cell behavior is a major challenge for lithium ion batteries. Focusing on liquid electrolytes, we describe parameter-free molecular dynamics predictions of their mass and charge transport properties. The simulations agree quantitatively with experiments across the full range of relevant ion concentrations and for different electrolyte compositions. We introduce a simple analytic form to describe the transport properties. Our results are used in an extended Newman electrochemical model, including a cell temperature prediction. This cross-scale approach provides quantitative agreement between calculated and measured discharge voltage of a battery and enables the computational optimization of the electrolyte formulation.

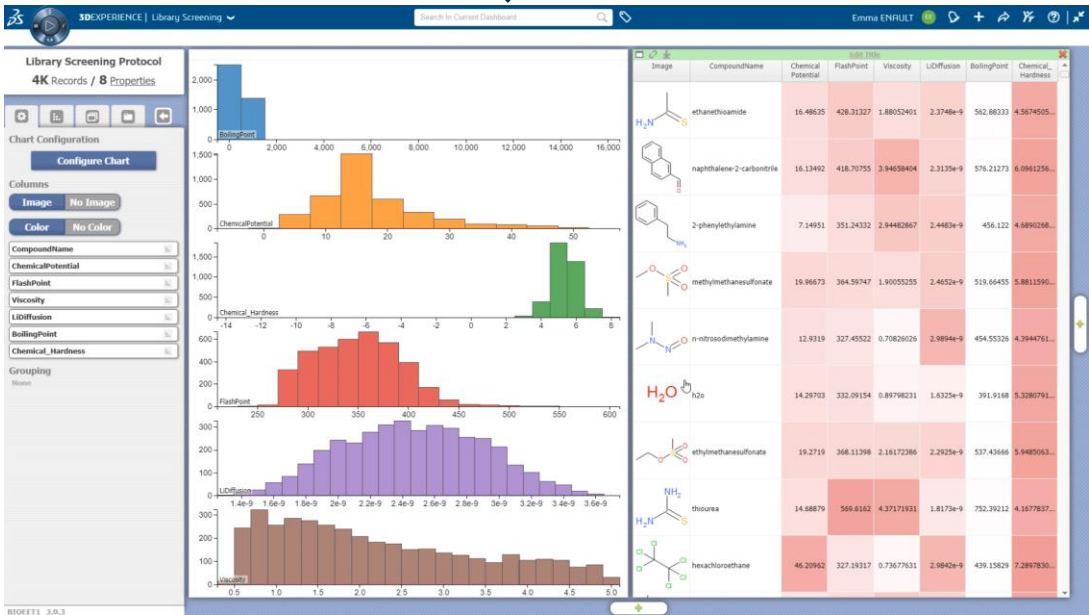
[DOI: 10.1149/2.0222001JES]

Hanke et al. J Electrochem Soc **167** 013522 (2020)

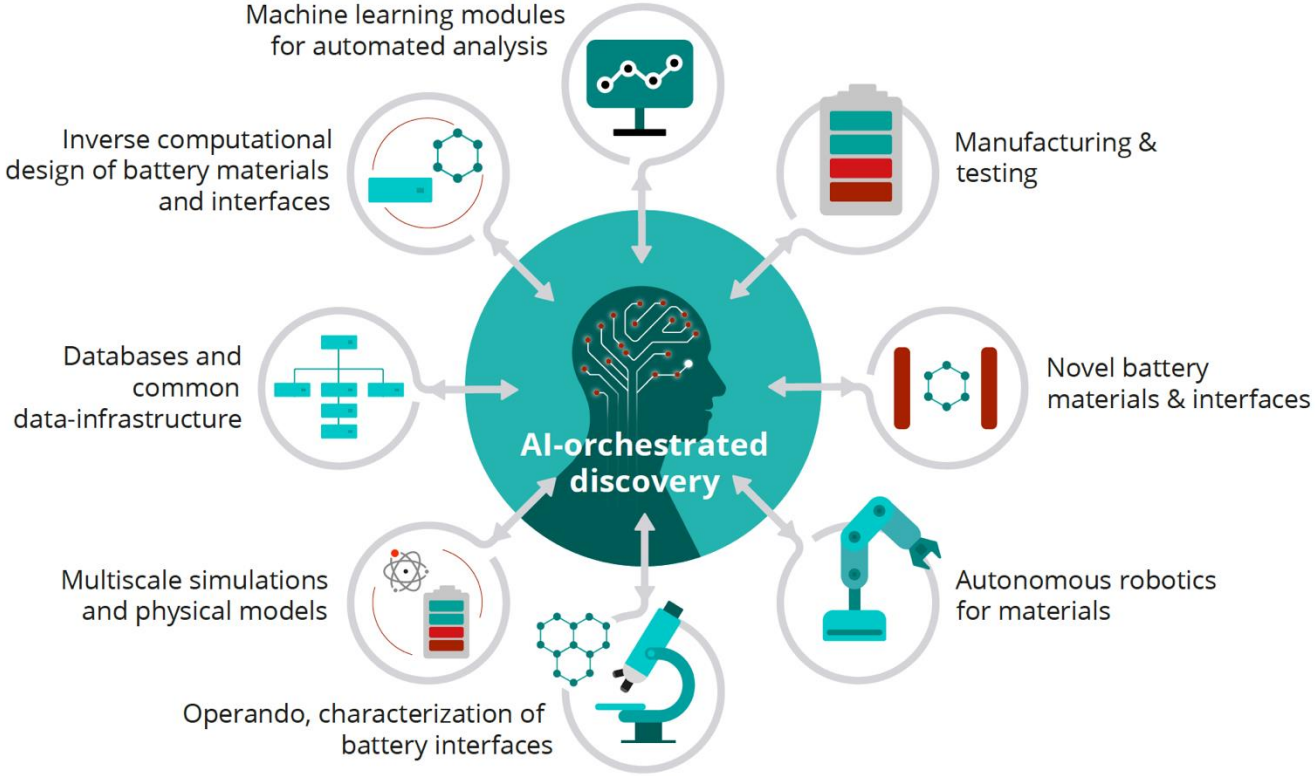
Battery demonstrator

- Set up and launch calculations
- Collect results
- Make analysis





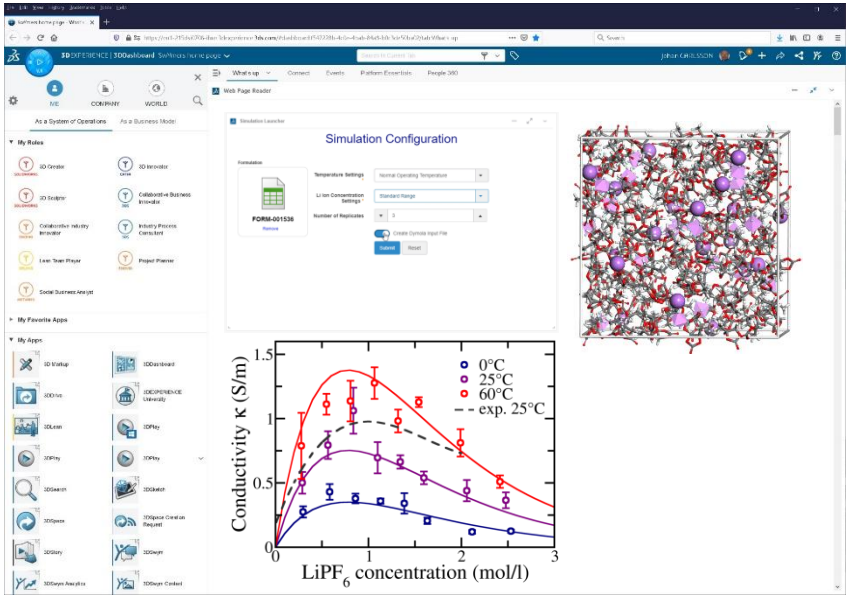
BIG-MAP Project Overview



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189.

3DS role in BIG MAP

- WP2: Demonstrator for training new force-field parameter sets for classes of battery materials.
- WP9: Infrastructure demonstrator for manipulation of BIG-MAP data inside 3DEXPERIENCE
- WP11: Demonstrator for training predictive models based on Machine Learning (ML) from simulation and experimental battery performance data



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BIG MAP benefits to Dassault Systèmes

BIG-MAP is a w**orld class experts network** in the battery field

Access to both **experimental and computational data and scientific results**

Demonstrate **scientific workflows in 3DEXPERIENCE platform** industrial software solution

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Defining scientific workflows suitable for battery materials discovery

Collaboration around data management and interpretation of data for battery tests

Testing new routes for battery materials discovery based on Artificial Intelligence

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