



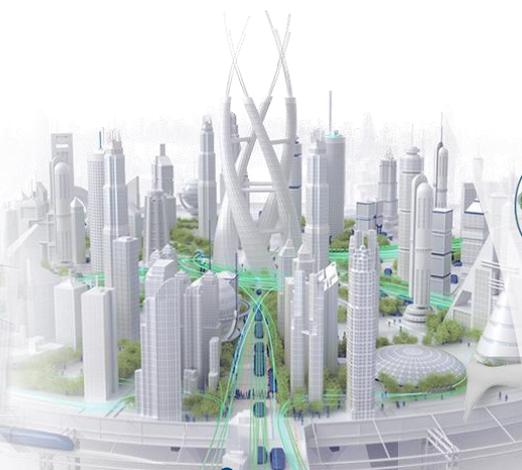
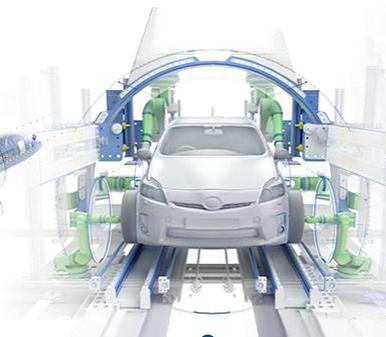
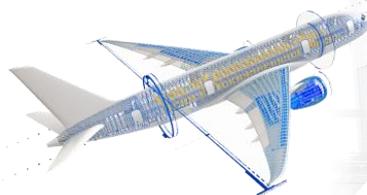
**3DEXPERIENCE**<sup>®</sup>

# 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 Systèmes



1981  
3D  
Design

1989  
3D DMU  
Digital  
Mock-up

1999  
3D PLM  
Product Lifecycle  
Management



2012  
3DEXPERIENCE®  
platform

2020  
Virtual Twin  
Experience  
of Humans

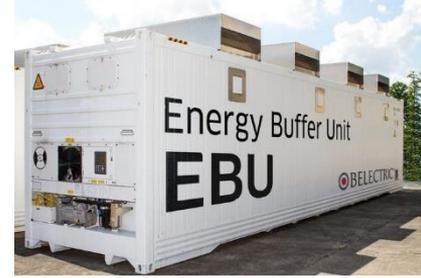


# Why is 3DS interested in Batteries?

- ▶ 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>



# Total Coverage From Chemistry To Systems

Molecular

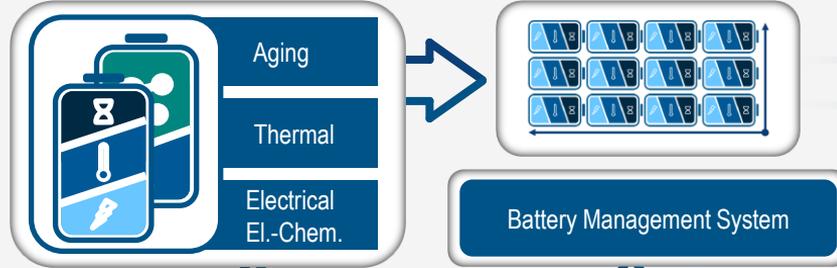
Cell

Module & Pack

Device

**Behavior Models**  
for System Design,  
Verification & Validation

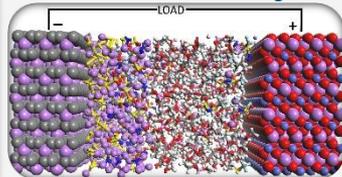
1D



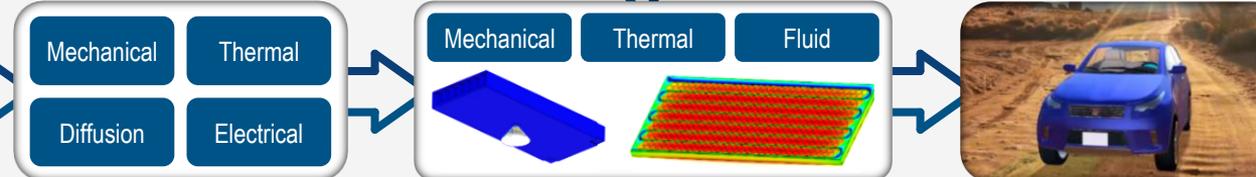
**High-Resolution Models**  
for Detailed Design & Analysis

3D

Molecular level material and chemical modeling



**3D. DESIGN | ENGINEERING | PHYSICS**

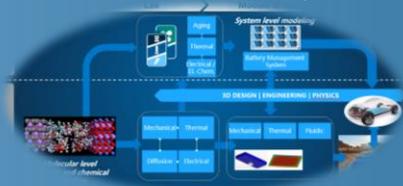


# 3DEXPERIENCE Platform enables the Industrialization of Sustainable Batteries



## 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

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

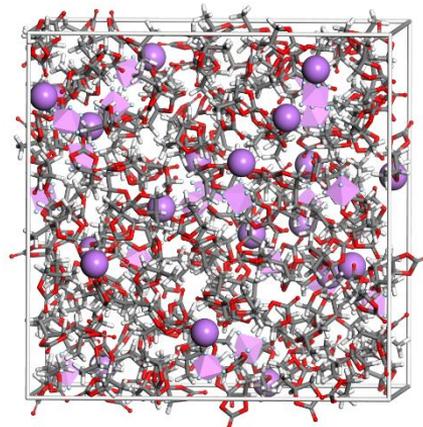
Establishing a link between atomistic processes and battery cell behavior is a major challenge for lithium ion batteries. Focusing on liquid electrolytes, we describe parameter-free molecular dynamics predictions of their mass and charge transport properties. The simulations agree quantitatively with 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. © The Authors 2019. Published by ECS. This is an open access article distributed under the terms of the Creative Commons Attribution 4.0 License (CC BY, <http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted reuse of the work in any medium, provided the original work is properly cited. [DOI: 10.1149/2.0222001JES]



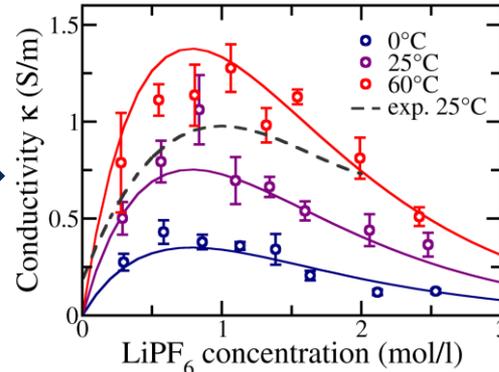
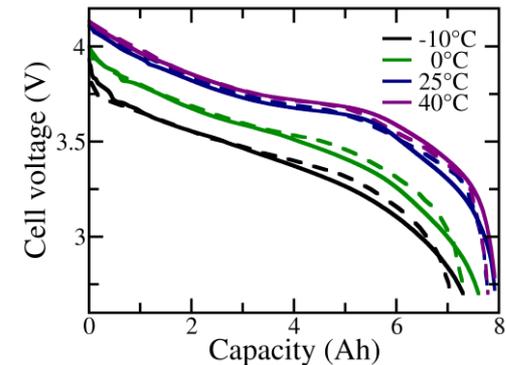
# Influence of Electrolyte Performance

## 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

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

# Battery demonstrator

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

Simulation Configuration

Formulation: FORM-001536

Temperature Settings: Normal Operating Temperature

Li Ion Concentration Settings: Standard Range

Number of Replicates: 3

Submit | Reset

3D Space: My Collaborative Spaces | Battery Project

Electrolyte Additives, FORM-001536, FORM-001537, FORM-001538, FORM-001539, NMC\_WLTP, NMC\_WLTP (Running)

Library Screening Protocol

4K Records / 8 Properties

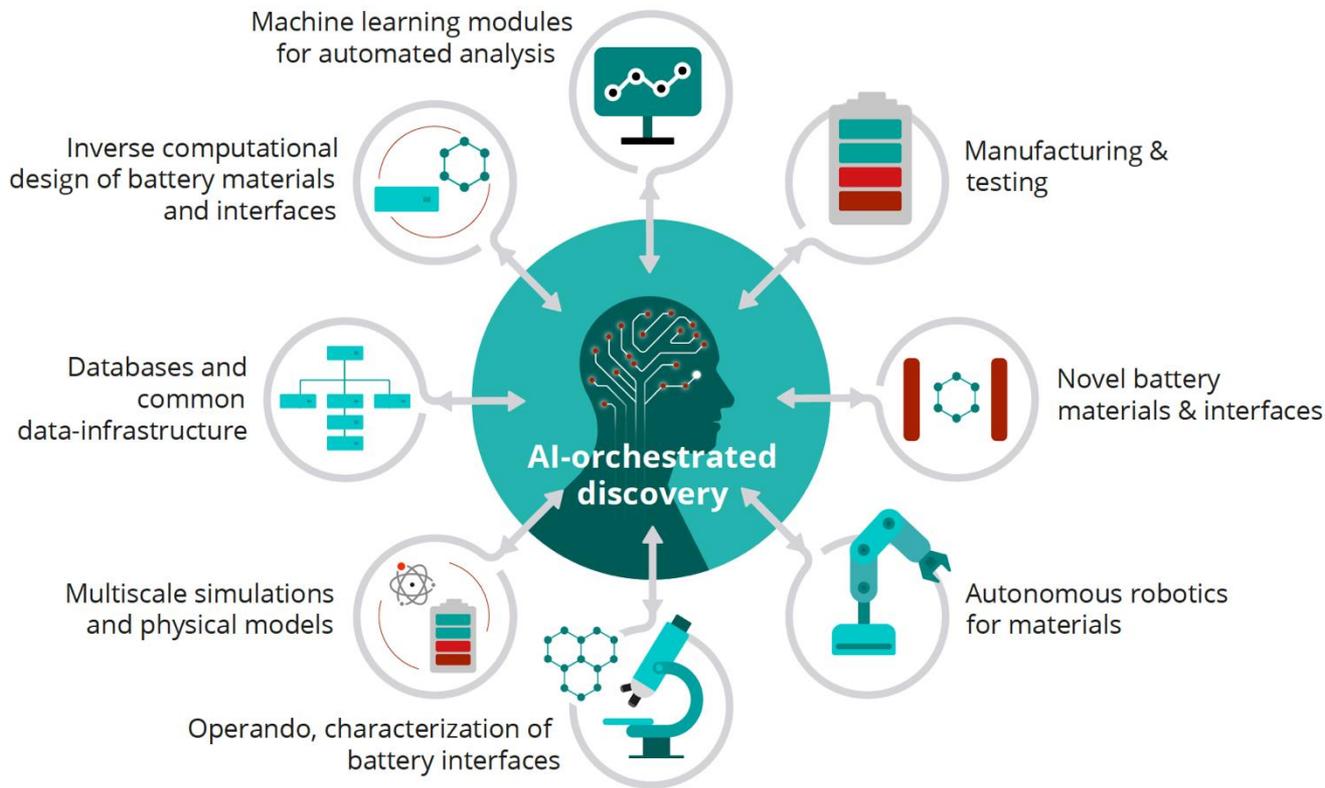
Chart Configuration

Columns: Image, No Image, Color, No Color

CompoundName, ChemicalPotential, FlashPoint, Viscosity, LDIffusion, BoilingPoint, ChemicalHardness

Image	CompoundName	Chemical Potential	FlashPoint	Viscosity	LDIffusion	BoilingPoint	ChemicalHardness
<chem>CC(=O)N</chem>	ethanamide	16.48635	428.31327	1.88052401	2.3746e-9	562.68333	4.5674505...
<chem>c1ccc(cc1)C(=O)N</chem>	naphthalene-2-carbonitrile	16.13492	418.70755	3.94658404	2.3135e-9	876.21273	6.0941256...
<chem>CCN(C)CC</chem>	2-phenylethylamine	7.14951	351.24332	2.84482867	2.4483e-9	456.122	4.6892568...
<chem>COS(=O)(=O)C</chem>	methylmethanesulfonate	19.96673	364.59747	1.90055235	2.4632e-9	519.66455	5.8812595...
<chem>CN(C)C</chem>	n-nitrosodimethylamine	12.9319	327.45522	0.70826026	2.9894e-9	454.55526	4.3944761...
<chem>O</chem>	H <sub>2</sub> O	14.29703	332.09154	0.89796231	1.6325e-9	391.91468	5.3280791...
<chem>CCOS(=O)(=O)C</chem>	ethylmethanesulfonate	19.2719	368.11398	2.16172386	2.2925e-9	537.43666	5.9485033...
<chem>NC(=O)N</chem>	thiourea	14.88879	569.6162	4.37171931	1.8173e-9	752.39212	4.187837...
<chem>CC1(C)CC1</chem>	hexachloroethane	46.20962	327.19317	0.73677631	2.9842e-9	439.15829	7.2867830...

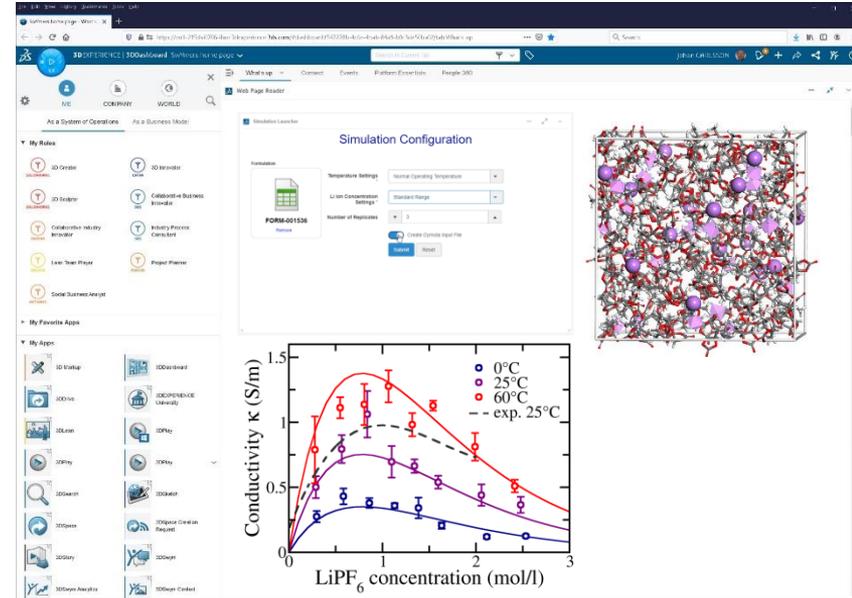
# BIG-MAP Project Overview



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



# BIG MAP benefits to Dassault Systèmes



BIG-MAP is a **world 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



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

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

