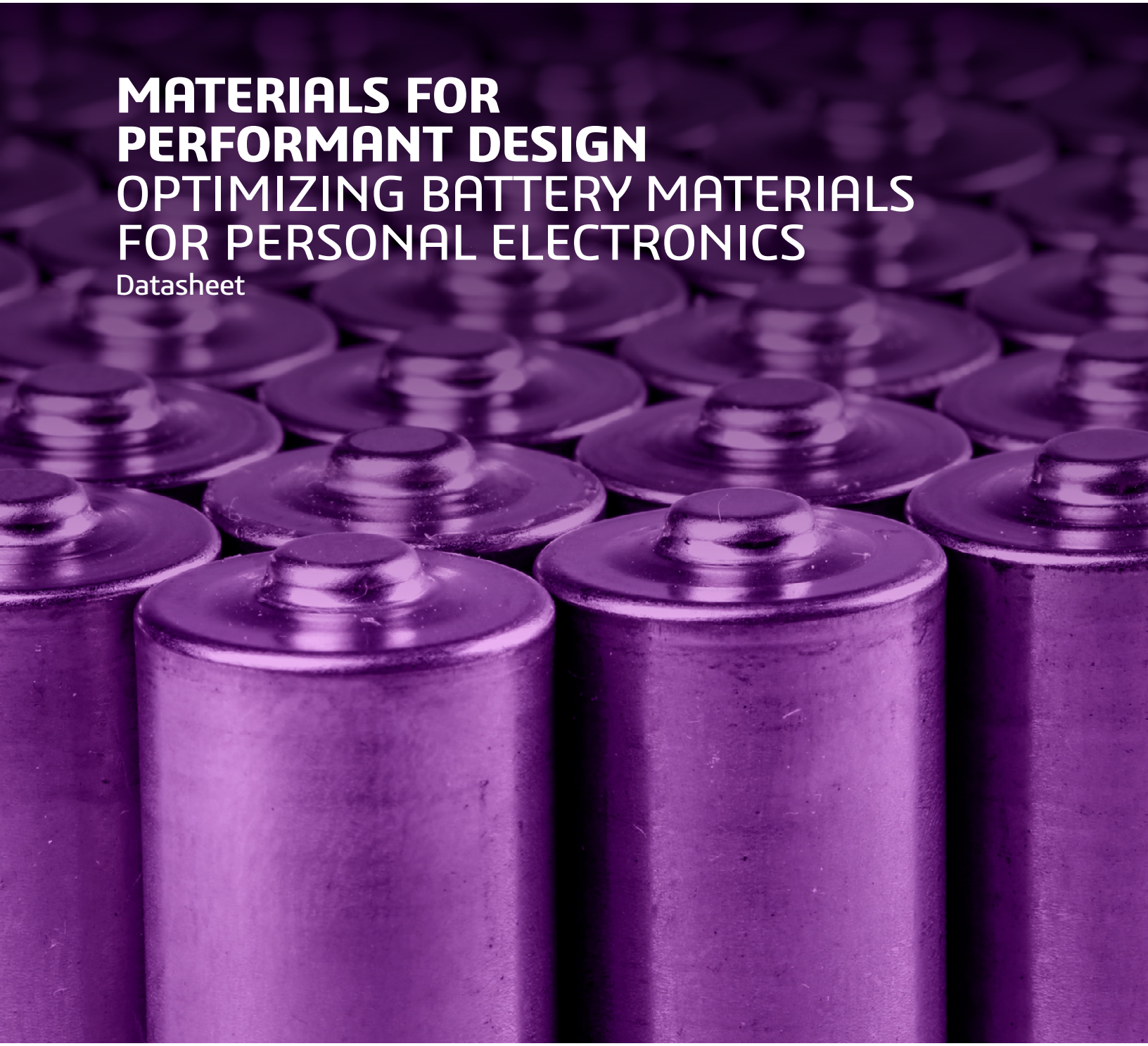
BIOVIA

3DEXPERIENCE®

MATERIALS FOR PERFORMANT DESIGN

OPTIMIZING BATTERY MATERIALS FOR PERSONAL ELECTRONICS

Datasheet



DASSAULT SYSTEMES

The technological advances of the past few decades have more often than not been powered by lithium-ion batteries (LIBs). While LIBs started in personal electronics such as mobile phones, in recent years the market has penetrated segments as diverse as medical devices and electric vehicles. The resulting growing number of use cases has thus produced a consummate growth in the demands for improved performance: LIBs must last longer, decrease in size, have greater capacity and become safer and more durable. This is pushing existing offerings to their limits, and some organizations are looking into fundamentally different materials to replace existing components to meet these challenges and improve production capacity. This is easier said than done, however, as LIBs rely on – and degrade by – a host of subatomic and intermolecular interactions. Fostering an understanding of these mechanisms and how they relate to battery performance requires that researchers and engineers look beyond physical experimentation alone. *In silico* modeling and simulation provides a way forward.

TIE INTERMOLECULAR INTERACTIONS TO MATERIALS BEHAVIOR

Materials for Performant Design from the Dassault Systèmes' BIOVIA brand provides a comprehensive suite of *in silico* methods for the characterization, prediction and optimization of LIB materials. These virtual methods can provide the foundation that researchers and engineers need to bring higher performance, more sustainable offerings to market at lower cost.

Anode

Key challenges for LIB batteries is extending their lifetime by increasing the number of charge and discharge cycles a cell can undergo before degrading and accelerating battery charging. Novel anode materials present an intriguing opportunity for achieving these goals. Existing materials such as graphite intercalate lithium ions to "store" them for discharging, but over time this cycle of expanding and contracting can lead to its breakdown. Additionally, the processes by which intercalation occurs can lead to "traffic jams" in the battery, slowing charging cycles. Materials for Performant Design can help researchers understand how anode materials work at the atomic level, helping them identify new materials such as silicon nanostructures and optimize their performance for various use cases.

- Improve anode durability by elucidating the atomic processes which lead to graphene exfoliation and overall anode degradation
- Extend anode lifetime by exploring the factors which control the growth and stabilization of the solid electrolyte interface
- Optimize anode performance by predicting how lithium ions arrange within the anode during charging and discharging
- Minimize the impact of metal dendrites and other issues on battery life by determining the atomic-scale mechanisms for their formation

Cathode

Ongoing research in cathode materials focuses primarily on identifying and optimizing materials that are relatively cheap while improving energy density and cycling stability such as $LiNi_xMn_yCo_zO_2$ or $LiNiCoAlO_2$. Materials for Performant Design can assist teams by simulating cycling, degradation and electrolyte interactions, helping ensure that teams are working on projects that are more likely to succeed on the market.

- Determine charging and discharging activity for various materials by calculating the Open Cell Voltage (OCV)
- Assess changes in cathode structure during cycling to determine its impacts on overall cathode capacity
- Explore and optimize the interactions between the cathode surface and various coatings to improve durability

Electrolyte

Battery safety remains a central concern for producers of LIBs, especially as the market places increasing scrutiny on failures. Often, the resulting fires are fueled by the volatile organic solvents such as dimethyl carbonate. To this end, many new projects are exploring reformulation of the electrolyte with additives that can raise the overall flash point of the system or are shifting the focus to solid electrolyte phases utilizing ceramics or zeolites. Materials for Performant Design provides a host of methods to characterize and optimize electrolyte behavior, helping teams mitigate safety risks further upstream in R&D.

- Calculate the diffusion of lithium ions throughout pure electrolytes or mixtures
- Investigate how electrolyte molecules are broken up and incorporated into the solid electrolyte interface during operation
- Determine the properties of electrolyte additives to assess how they influence the performance
- Predict the viscosity of electrolyte formulations
- Predict the safety of electrolytes based on properties like vapor pressure and flash point

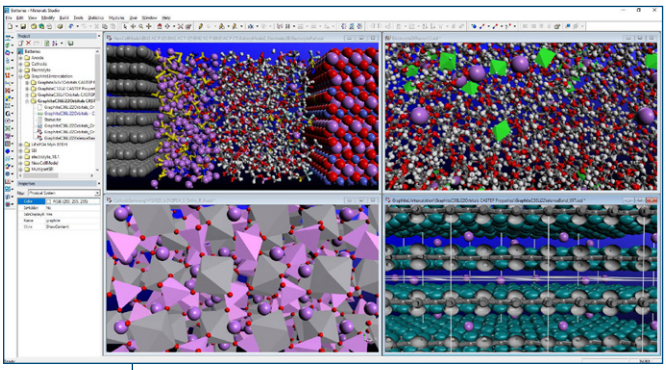


Figure 1. Depictions of simulations of Li-ion battery components.

FROM CHEMISTRY TO SYSTEM

The broader portfolio from Dassault Systèmes allows for further characterization of battery components, providing a truly multiscale solution for their design. With this information, researchers and engineers can better understand how these new materials can perform "in action," guiding future work to improve their safety and overall electrochemical performance.

- Utilize existing simulation results to parameterize calculations within SIMULIA Abaqus to perform 3D simulations of thermal and mechanical properties of battery cells
- Run system-level simulations of the performance of battery cells with CATIA Dymola Battery Library

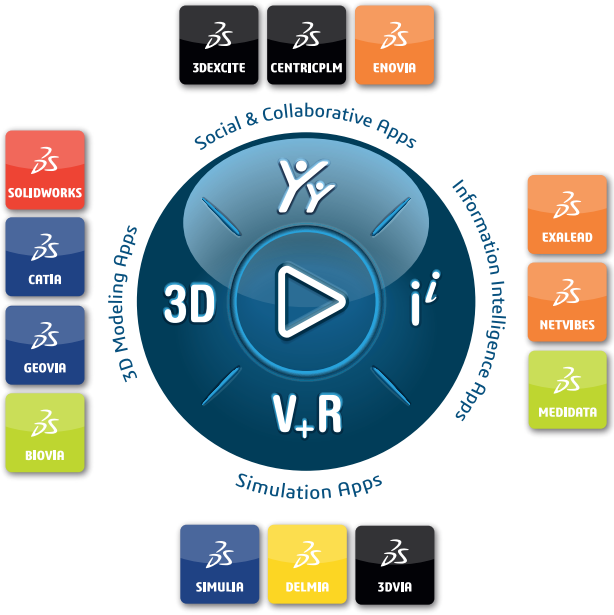
PRODUCING SAFER, MORE POWERFUL BATTERIES

The increasing preponderance of electronics is transforming the ways people go about their daily lives, and LIBs are powering this change. As organizations look towards the future of power storage, they will need to increasingly adopt modern solutions to augment their R&D efforts. The insights offered by Materials for Performant Design from BIOVIA will allow researchers and engineers to probe the fundamental interactions that underpin battery behavior, guiding the design of materials and devices that are safer, longer-lasting, and more sustainable.

Our **3D**EXPERIENCE® Platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3D**EXPERIENCE platform and applications, our customers push the boundaries of innovation, learning and production.

Dassault Systèmes' 20,000 employees are bringing value to more than 270,000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit **www.3ds.com**.



DASSAULT SYSTEMES | The **3D**EXPERIENCE® Company

Europe/Middle East/Africa
Dassault Systèmes
10, rue Marcel Dassault
CS 40501
78946 Vélizy-Villacoublay Cedex
France

Asia-Pacific
Dassault Systèmes K.K.
ThinkPark Tower
2-1-1 Osaki, Shinagawa-ku,
Tokyo 141-6020
Japan

Americas
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA