BIOVIA

3DEXPERIENCE®

CONTRACT RESEARCH – AN OUTCOME BASED ENGAGEMENT TO DESIGN, OPTIMIZE, INNOVATE BATTERY CELLS

Datasheet

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 electric vehicles, hybrid and electric aircraft, medical devices (including surgical power tools, wearables, pacemakers, critical care devices, etc.), and many more. The growing number of use cases has thus produced a consummate growth in the demands for improved performance: LIBs must last longer, decrease in size and weight, have greater capacity, become more affordable, and more sustainable while becoming safer and more durable. This is pushing existing offerings to their limits, and many organizations are looking into improving the materials, searching a large phase space of materials, coatings, process conditions, etc., to replace existing components and processes to meet these challenges and improve production capacity. This is easier said than done, however, as LIBs are activated and used, they degrade by a host of chemical and electrochemical reactions fundamentally driven by inherent materials characteristics such as electronic features, atomistic structures, intermolecular interactions, nano and microporosity, mechanical and thermal stability, etc.

An in-depth understanding of mechanisms involved in activation, charge/discharge usage cycles, and cell degradation is identified as the key to achieving a competitive edge. Battery cell manufacturers, niche cell designers, and materials companies are vying to get to this "root cause" and gain critical insights in their intense race to the top. All want to leverage virtual twin approaches to accelerate towards their goals so they can achieve and maintain leadership and increase market share in a very competitive area with very aggressive time scales.

DASSAULT SYSTEMES is uniquely positioned to enable this transformative change by leveraging its expertise in a multidisciplinary, multi-paradigm, and multiscale outcome based Contract Research engagement model. Advanced and next-generation batteries, whether it is Li metal or Si-based anodes, solid-state electrolytes with ceramics, polymers, or hybrids, advanced Li-ion designs, Li-S, Na-ion, redox flow batteries, Al-air, Na-air, Zn-air, low to no Co cathodes, and a multitude of other chemistries and processes can be investigated in-depth virtually with the help of Dassault Systèmes Contract Research battery solutions. This enables the industry to accelerate by 30% or more towards its goals.

DASSAULT SYSTEMES

CONTRACT RESEARCH – A STRATEGIC COLLABORATION TO BRIDGE THE GAP

Contract Research from Dassault Systèmes provides a collaborative approach where, under strict confidentiality, we become an extended arm of our customers' battery research, development, and innovation lab. Focused on the goal of our customers, we bring together the right multidisciplinary expertise and the most appropriate set of software tools to address the critical scientific and engineering challenges of our customers. **Contract Research** engagements with our customers are action-focused research with outcomes that drive real-time decisions and accelerate innovation. This close collaboration between our computational experts and customer's experts (consisting of the experimental lab team and the engineering modeling team) makes for a very successful outcome. **Contract Research** battery domain experts have developed Advanced Technology Capability (ATC) based on BIOVIA software (including modeling & simulation tools and machine learning tools) that covers battery-specific validated models, and scientific algorithms beyond those already available in the software tools, domain-specific content (data), and validated workflows. This comprehensive suite of ATCs in the hands of our domain experts allows them to address the challenging and business-critical scientific problems of our industrial customers efficiently. Outcomes from such engagements can range from accelerated design and predictive modeling, focusing experiments for success, root-cause analysis of failure modes with potential remedial measures, virtual design-of-experiments, critical insights that provide "know-why", and last but not the least a connection to macroscale cell engineering models. Figure 1 shows how **Contract Research** bridges the gap between software tools and industries' end goals for the next generation battery which is more durable and has higher capacity while being sustainable and safer.

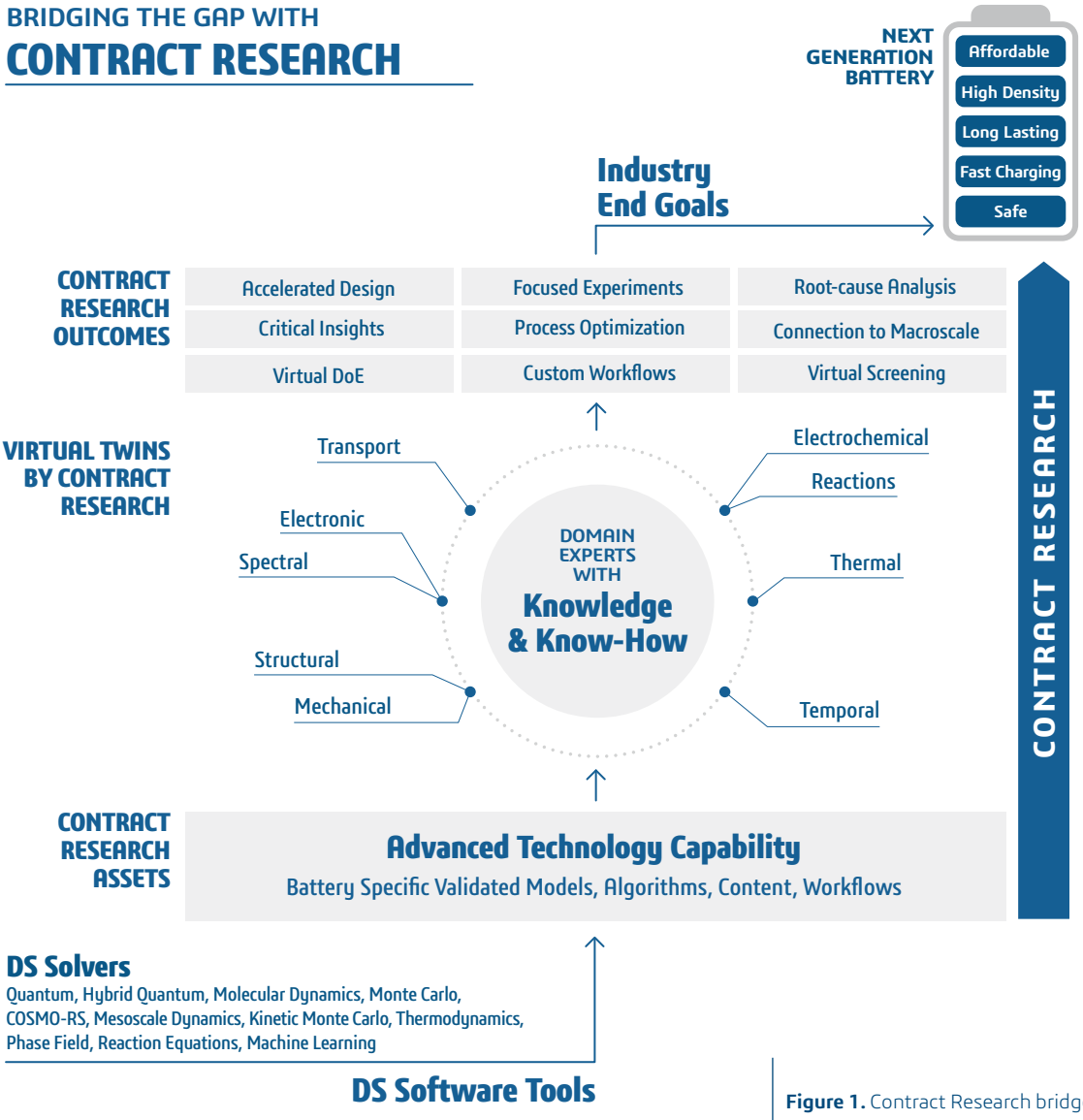

Figure 1. Contract Research bridges the gap between software tools and industry end goals for the next generation battery.

TIE MATERIALS CHEMISTRY TO BATTERY CELL BEHAVIOR

BIOVIA provides molecular modeling and simulation tools in the areas of quantum mechanics, hybrid quantum mechanics, molecular dynamics, COSMO-RS, mesoscale dynamics, kinetic Monte Carlo, phase field, and rate equations. A combination of these tools and other characterization tools in BIOVIA's Materials Studio suite provides the foundation. Built on this base, the ATCs then are used to create virtual twins of the battery sub-component and simulate the processes. **Contract Research** has bridged the gap connecting materials chemistry to battery life, safety, performance, and end-of-life aspects Topics such as cell activation, chemical, electrochemical, and thermal processes during cycling, impact due to external conditions, usage-based effects, as well as ageing processes can now be investigated in-depth.

Anode

A key challenge for LIB batteries is to meet the growing demands of smaller and lighter rechargeable batteries that can still deliver high capacity. Metallic Lithium has a low density and a high theoretical specific capacity. If some of the failure modes are tackled in a cost-effective manner, this will make Li metal batteries (LMBs) the ideal for the next generation products. **Contract Research** can help battery developers to design, optimize and innovate better performing anodes from a "model-first" approach. With validations done at every stage with experimental analytical measurements and lab tests, we accelerate efforts towards the most successful experiments.

- Optimize anode performance by predicting lithiation and delithiation within the anode during charging and discharging cycles
- Design anode coatings for faster and improved solid electrolyte interface (SEI) durability
- Suppress dendrite formation and swelling, by root-cause analysis approaches

Cathode

Ongoing research and development of cathode active materials focuses primarily on identifying and optimizing materials that are relatively lower cost, easier to obtain, and at the same time improve energy density and cycling stability. **Contract Research** enables battery manufacturers in many ways, some of them are listed here.

- Virtual design-of-experiments (DoE) to tune the mixing, drying, and calendering process
- Determine charging and discharging activity for various materials by calculating the Open Cell Voltage (OCV)
- Assess changes in cathode structure during cycling to determine the impact on overall cathode capacity
- Explore and optimize the interactions between the cathode surface and various coatings to improve durability

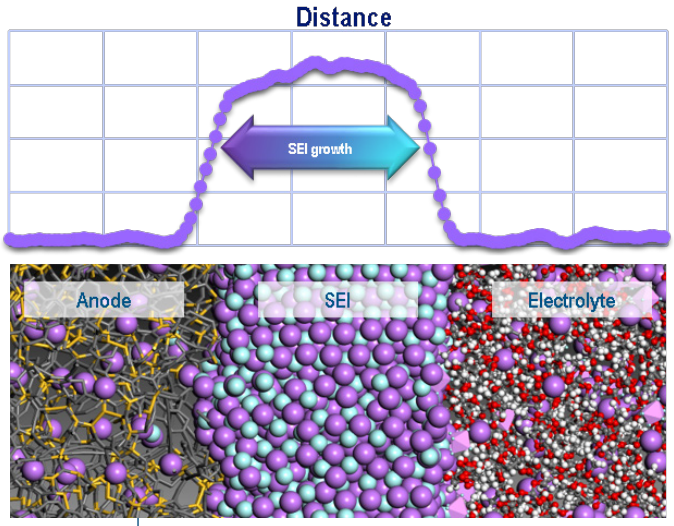

Figure 2. Electrochemical reactions of the electrolyte during the activation stage of manufacturing results in SEI growth. Using Advanced Technology Capability validated models and content, Contract Research is able to simulate the process of SEI growth from first-principles modeling and simulations.

Electrolyte

Battery safety remains a central concern for producers of LIBs. To this end, the industry is shifting the focus to solid-state electrolytes (SSE). Industry has turned to DASSAULT SYSTEMES' **Contract Research** to address these challenges.

- Apriori calculation of conductivity, transference number, and diffusion of Li ions in the electrolyte
- Validated models of SEI formation and growth based on the electrolyte used completely from first principles
- Virtually screening numerous electrolytes, additives, and formulations to select the most promising candidates and formulations to be tested in the lab

Machine Learning & AI Applied to Predict Performance of Battery Cell

For Machine Learning and data science, the very versatile tool Pipeline Pilot is available from BIOVIA. Based on this, **Contract Research** has created Advanced Technology content and validated models. Using customer-proprietary data, these models can be further tuned for customer-specific systems. In addition, we have also applied this expertise to predict battery lifetime and performance based on the first few cycles of experimentally measured data.

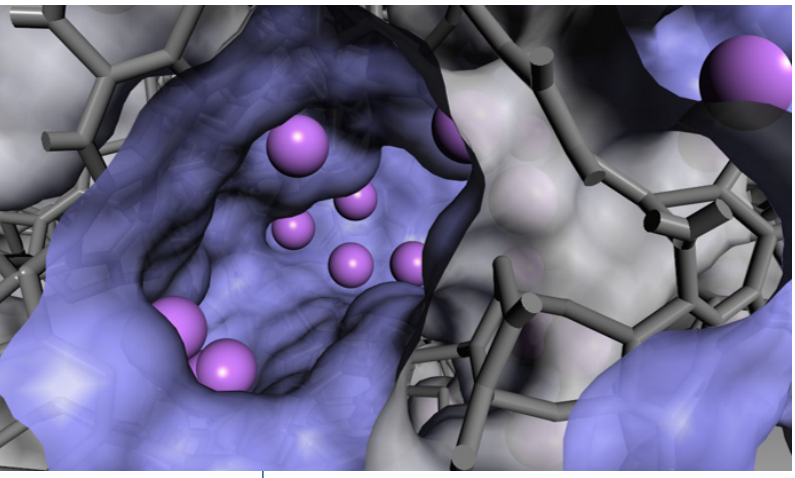

Figure 3. Using Advanced Technology Capability validated algorithms and workflows, Contract Research is able to model the ion transport in a solid state electrolyte in the absence of any prior experimental data.

FROM ELECTRONS TO ELECTRIFICATION

The broad portfolio from Dassault Systèmes allows multiscale, multidisciplinary, and multiple paradigm-based virtual twin for a model-first approach in the design, optimization, and innovation of battery sub-cell materials and components, cell design, pack and module design, and manufacturing. **Contract Research** provides the expertise to apply our technology to critical challenges that our customers face.

CONTRACT RESEARCH ENABLES LIGHTER, FASTER, BETTER, CHEAPER, SAFER BATTERIES TO REACH SUSTAINABILITY GOALS

The increasing preponderance of electronics is transforming the way people go about their daily lives, and LIBs are powering this change. As industries improve and innovate batteries for EVs, eVTOL, power storage, personal electronic devices, medical devices, etc., they have realized the power of an end-to-end virtual twin to cut down waste, decrease experiments and focus them towards the most successful paths, accelerate time-to-market for next-generation products, and gain a competitive edge. **Contract Research** is the go-to team in DASSAULT SYSTEMES for the needs of the industry ranging from mining, energy and materials, transportation and mobility, high technology, and medical devices. Through a strong partnership established in **Contract Research**, the best teams are formed by bringing together experts. The strict confidentiality and mutually beneficial IP terms, and timely delivery of goal-focused milestones by **Contract Research** is the perfect formula for a winning collaboration to create next-generation batteries which are lighter, faster, better, cheaper, safer, and also more easily recyclable.

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

Dassault Systèmes, the **3DEXPERIENCE** 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 **3DEXPERIENCE** 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**.

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

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

DS-10004-0422