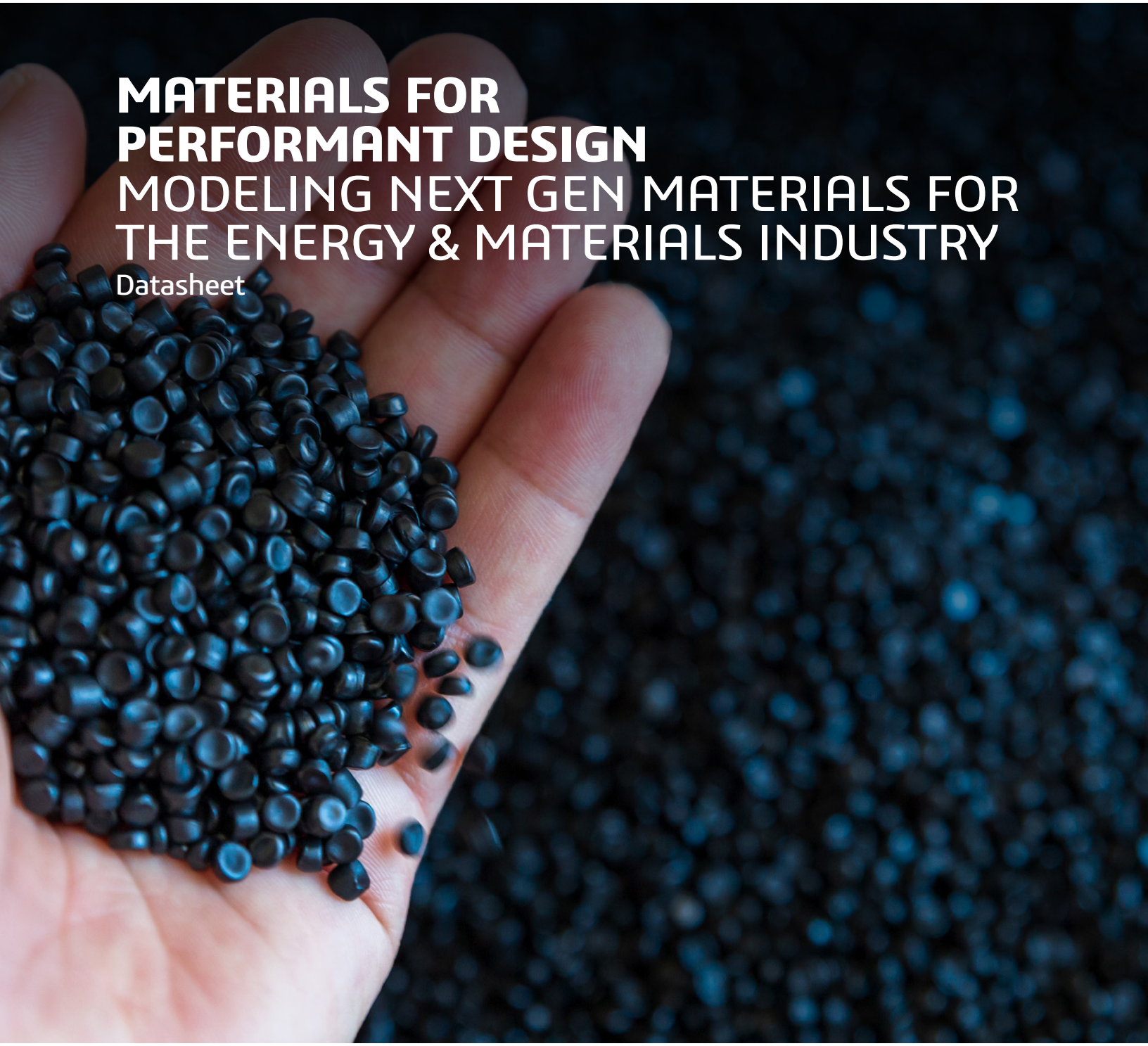
BIOVIA

3DEXPERIENCE®

MATERIALS FOR PERFORMANT DESIGN

MODELING NEXT GEN MATERIALS FOR THE ENERGY & MATERIALS INDUSTRY

Datasheet



DASSAULT SYSTEMES

Today's Energy & Materials (E&M) companies are facing growing pressure to embrace sustainability and demands to produce offerings for increasingly targeted markets. As a result, teams are looking to improve operational efficiency, especially in R&D. This specialization, however, requires a deep understanding of the fundamental properties of a host of formulated products and pure materials: catalysts, polymers, composites, lubricants, coatings and specialty chemicals. Relying on physical experimentation alone to foster this understanding is proving to be insufficient to keep up with market and regulatory demands. To succeed, E&M organizations will need to more thoroughly embrace other approaches and techniques. *In silico* modelling and simulation and machine learning techniques can provide the needed foundation for teams to bring high quality offerings to market faster and at lower cost than ever before.

FOSTERING UNDERSTANDING OF MATERIALS BEHAVIOR

Materials for Performant Design from Dassault Systèmes' BIOVIA brand offers a complete suite of *in silico* techniques and machine learning capabilities to allow researchers to probe the intermolecular interactions that underlie materials properties.

Catalysts

Improving the energy efficiency and specificity of chemical processes remains a key consideration for E&M companies; even marginal gains can net millions in savings annually. Identifying and optimizing catalysts that are fit-for-purpose lies at the heart of these efforts. Yet doing so for increasingly specific projects and offerings requires that teams deepen their understanding of the molecular mechanisms that impact their catalysts' activity and the reaction pathways that produce their end products. With Materials for Performant Design, researchers can probe this behavior, accelerating the next collection of catalysts to full scale production.

- Screen new catalysts based on their chemical structures via statistical and Machine Learning methods
- Locate the most stable adsorption sites in materials such as zeolites
- Calculate the impacts of local geometries and/or defects on the catalyst's mechanism of action
- Characterize the electronic and chemical properties of metal-ligand complexes
- Predict catalyst structure and properties for large systems such as nanoparticles (>500 atoms)
- Predict reaction energies, activation barriers, and kinetic rate constants
- Conduct simulations of chemical reactions taking place at crystal surfaces
- Predict concentrations of reactants and products under various reactor conditions and geometries

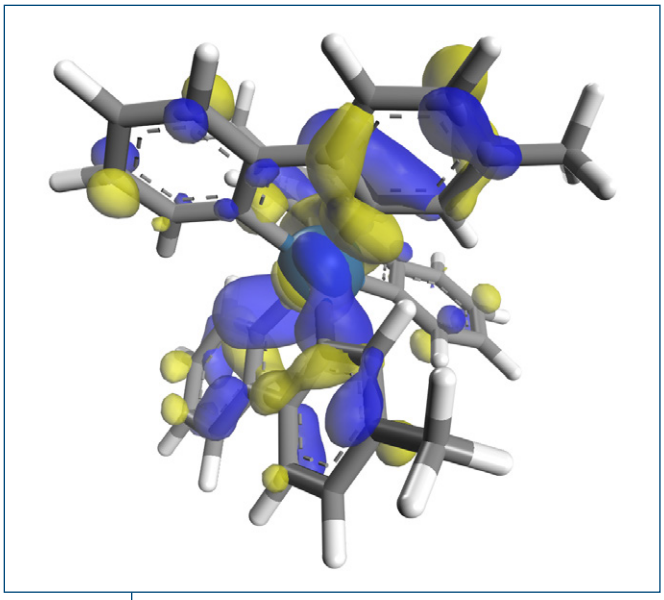


Figure 1. The electronic structure of a metallocene catalyst.

Polymers & Composites

The versatility of polymer and composite materials have led to their widespread adoption for a variety of end uses, from water bottles to aircraft fuselages. However, concerns around their impact on the environment are pushing efforts to improve recyclability and utilize alternate feedstocks and production methods for sustainability. Meeting these requirements hinges on understanding how these processes can influence polymer properties such as chain length and tacticity; how a polymer's chemical structure influences its mechanical properties and degradation pathways; and how blends, additives and fibers interact. Materials for Performant Design can help guide the R&D surrounding the development of more biodegradable polymers and composites and other sustainability efforts, allowing organizations to maintain high quality offerings while taking care of our planet.

- Predict the behavior of pure polymers and their physical properties such as glass transition temperature (Tg), Young's modulus, yield stress and critical strain
- Crosslink simulation to understand polymer network formation and impact of chemical structure, additives and processing on mechanical properties and their stability
- Calculate reaction energies and kinetics of polymerization and degradation reactions
- Use Quantitative Structure-Property Relationship (QSPR) models to correlate polymer repeat unit structure with bulk properties
- Cohesive strength and mechanical failure of the polymer-filler interface

- Screen sizing agents for production of carbon fibers of desired shape and size
- Simulate crosslinking of resin around the fibers and characterize the structure and binding strength

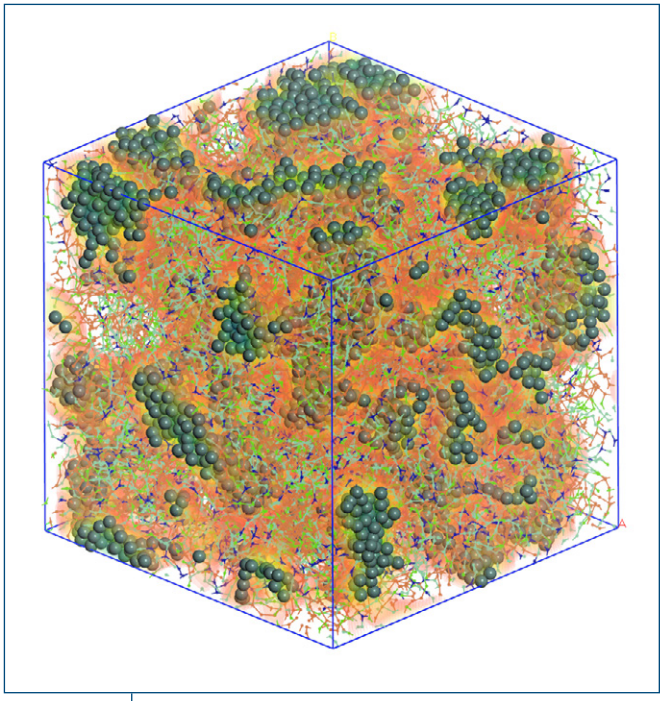


Figure 2. A model of the interactions of a polymer resin with various tougheners added

Lubricants, Coatings & Specialty Chemicals

High performance parts for automobiles, airplanes and electronics require equally specialized lubricants and coatings to protect them in the extreme conditions they operate in. Characterizing the atomic and molecular interactions that underlie this behavior quickly and efficiently remains a key challenge for many E&M providers, especially considering the pressure to design tailor-made offerings. Materials for Performant Design can expand the scope of these specialized R&D projects, ensuring the products that make it to market not only meet their design requirements, they exceed them.

- Improve product performance with predictive models which correlate molecular descriptors to materials properties
- Enhance coating durability by understanding surface chemical processes such as absorption and corrosion at the atomic scale
- Utilize machine learning to accelerate the identification of new candidate molecules and mixtures by predicting various bulk properties

PRODUCING TAILOR-MADE, MORE SUSTAINABLE PRODUCT LINES

The push for greener industrial operations and products is only increasing. Additionally, as downstream customers continue to develop higher performance planes, automobiles and electronics, E&M companies will need to offer equally high performing products that are fit-for-purpose. Understanding the "how and why" behind their materials' and formulations' behavior at the atomic level can accelerate this push. Materials for Performant Design can provide the insights that E&M researchers need to foster this understanding, paving the way to designing safer and more sustainable products for targeted use cases faster and at lower cost than ever before.

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