INDUSTRY APPLICATION

Driving Innovation in Polymer R&D with Molecular Simulation & Machine Learning

R&D scientists across broad industries from aerospace to electronics face challenges in developing the next-generation of polymers and composites with high-performance, multifunctional capabilities that also meet society's demands for miniaturization and environmental sustainability.

Schrödinger | Materials

Solution Overview

Chemical reactivity, physical morphology, and polymer physics drive the behavior of polymers and soft materials. Schrödinger's Materials Science platform provides a unique combination of capabilities for the design and optimization of polymers, including:

- Differentiated model builders
- Extremely efficient, GPU-powered molecular dynamics (MD) engine
- Automated thermophysical and mechanical response workflows
- Chemically adaptable cross-linking workflows
- Analysis tools for the simulation, optimization, and discovery of novel polymers including linear, crosslinked, elastomers, dendrimers, and copolymers

Schrödinger's tailored solutions for molecular modeling of polymers, mixtures, and composites can reduce cost and risk, shorten timelines and drive innovation in a broad range of industries.

Industries and Applications

Automotive and Aerospace

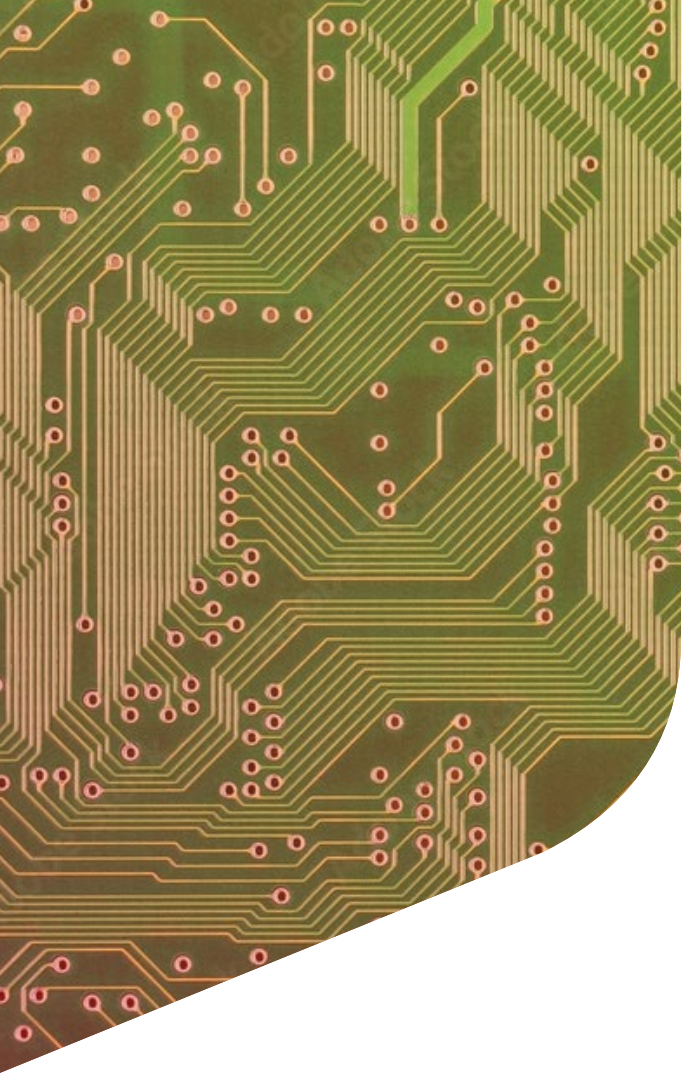
- **Optimize polymer formulation properties:** Model water transport, uptake and morphological stability in polymer composites using multistate simulations
- **Accelerate chemical design to properties critical to product and processing constraints:** Identify the unique combinations of epoxy-amine reactions for target properties using high-throughput screening
- **Accelerate the manufacturing process pipeline:** Predict polymer gelling during manufacturing process
- **Design greener products that are more environmentally sustainable:** Simulate and predict properties of high-performance resins with bio-based materials, and automate discovery of new biomaterials

CPG Packaging and Formulation

- **Develop environmentally sustainable packaging:** Study interfacial interactions between packaging materials and consumer goods, and simulate water uptake for barrier design and performance
- **Optimize polymer formulation:** Quantify the diffusion of additives in polymer packaging materials
- **Minimize production waste:** Understand the potential causes and impact of polymer production deviations
- **Innovate with natural materials:** Explore active, recyclable, and bio-based materials through molecular simulation
- **Reduce processing cost:** Evaluate new formulations for potential manufacturing challenges

Specialty Polymers

- **Speed up decision-making on catalyst selection for raw materials production:** Simulate and understand the catalysis mechanisms, selectivity, and reactivity of epoxy amine, urethane, and other reactions
- **Optimize the design of high-performance polymers:** Predict glass transition, thermal stability, and thermal expansion with new polymers
- **Drive innovation in polymer reactions:** Predict curing kinetics and processing properties

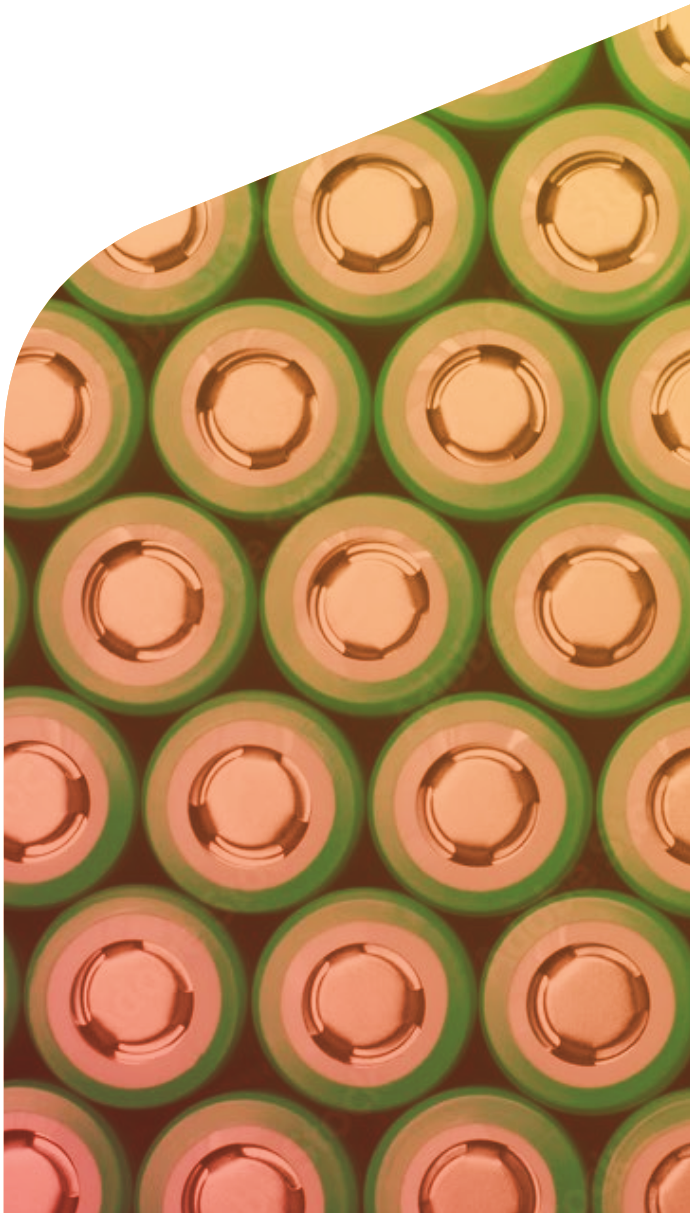


Electronic Packaging

- **Identify thermal/mechanical performance issues early in design:** Simulate coefficient of thermal expansion for packaging polymers
- **Optimize chemical stability:** Simulate interactions of packaging polymers with processing solvents and water to predict stability in use
- **Design new monomers for improved performance:** Predict design drivers like D_k, D_f and refractive index with physics-based simulations and machine-learned models

Batteries

- **Understand mechanisms at molecular level:** Predict electrolyte degradation reaction mechanisms and control energetics to understand the formation of functional solid electrolyte interphase layers at anodes (SEI) and cathodes (CEI)
- **Identify best-performing battery materials:** Perform high-throughput screening of anode, cathode, electrolyte and additive materials to identify best chemistries for development of next-generation batteries
- **Optimize electrolyte design:** Simulate interatomic interactions and transport of ions in liquid and polymer electrolytes



Pharmaceutical Formulation

- **Optimize drug carrier design**: Evaluate the solubility/miscibility of drugs with different polymeric carriers or barriers
- **Optimize drug formulations:** Visualize and characterize pH-dependent polymeric surfactant and drug interactions in solution and precipitation inhibition behavior
- **Drive effective drug delivery:** Simulate drug release profiles from amorphous solid dispersions into solution

Team Collaboration and Digital Data Management

- **Empower collaboration:** Employ web-based enterprise informatics tools for sharing experimental and predictive models seamlessly
- **Amplify research:** Rapidly deploy of machine learning models to drive predictions and assist novel design approaches
- **Improve project management:** Accelerate project communication and collective learning by capturing, analyzing, and testing new ideas and data in a centralized platform

Products

Check on the products that enable your success in the polymer industry.

Desmond

Highly efficient Molecular Dynamics (MD) tool

AutoQSAR

Automated machine learning tool

MS CG

MD tool with coarse-grained (CG)/mesoscopic sites

MS LiveDesign

Web-based enterprise informatics for materials design

OPLS4

Advanced modern force field

MS Dielectric

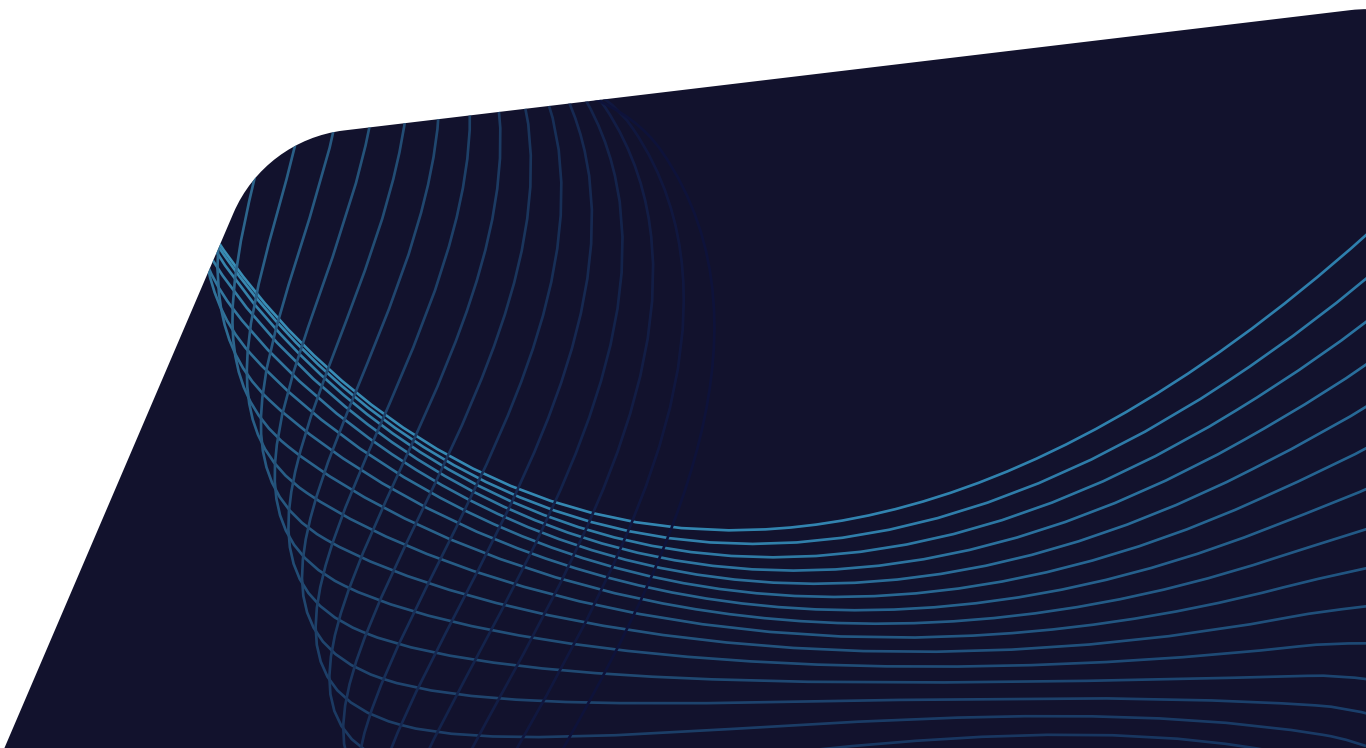
Combined QM & MD workflows for dielectric properties

MS Transport

MD workflows for shear viscosity, and the isotropic and anisotropic diffusion coefficients

MS Penetrant Loading

MD tool for prediction of water or small penetrant uptake



Selected Publications

Melt-state degradation mechanism of poly (ether ketone ketone): the role of branching on crystallization and rheological behavior.
Wiggins J. et al. *Polym. Degrad. Stab.* 2022, 200, 109968

Atomistic Molecular Dynamics in PEO/PMMA Blends Having Significantly Different Glass Transition Temperatures.
Habasaki J, *Int. J. Appl. Glass Sci*, doi.org/10.1111/ijag.16553

Experimental Investigations of AlMg3 Components with Polyurethane and Graphene Oxide Nanosheets Composite Coatings, after Accelerated UV-Aging.
Murariu A. C. et al. *Molecules* 2022, 27, 1, 84

Polycyanurates via Molecular Dynamics: In Situ Crosslinking from Di(Cyanate Ester) Resins and Model Validation through Comparison to Experiment.
Moore L. M. J. et al. *Macromolecules* 2021, 54, 13, 6275–6284

Photophysical Properties of Cyclometalated Platinum(II) Diphosphine Compounds in the Solid State and in PMMA Films.
Anderson C. M. et al. *ACS Omega* 2021, 6, 42, 28316–28325

High-Throughput Molecular Dynamics Simulations and Validation of Thermophysical Properties of Polymers for Various Applications. Afzal. A et al. *ACS Appl. Polym. Mater.* 2021, 3, 2, 620–630

Fundamental Limits to the Electrochemical Impedance Stability of Dielectric Elastomers in Bioelectronics.
Floch P. L. et al. *Nano Lett*. 2020, 20, 1, 224–233

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