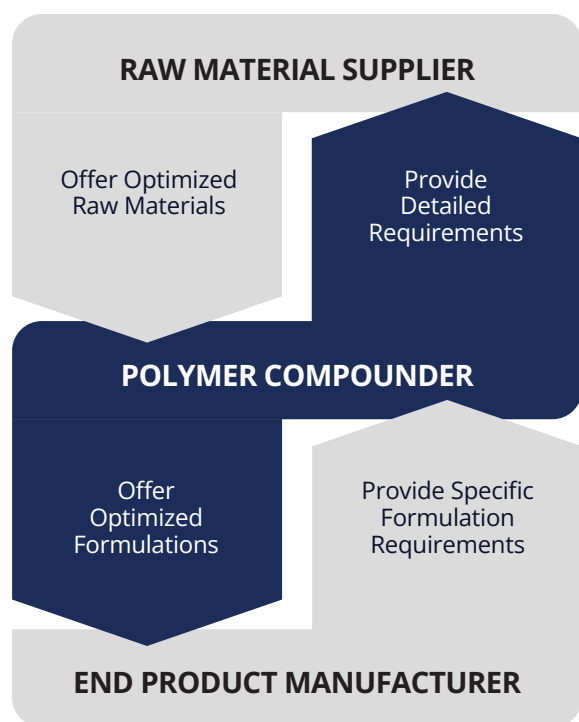


# The Role of Digital Chemistry Across the Polymer Supply Chain

Molecular modeling and simulation tools have proven effective in materials development and are increasing in use throughout the polymer industry, from raw materials suppliers to end product manufacturers. Computational workflows also open new avenues for developing polymers with improved recyclability. Physics-based simulations offer reliable predictions of structures, morphologies, properties, and chemical reactivity for polymers. Recent advances in machine learning, deep learning, and enterprise informatics platforms have accelerated the speed, accuracy, and automation of novel materials and solutions discovery. A paradigm shift to computer-driven molecular design is occurring throughout the industry.



## Vision of a digital chemistry catalyzed polymer supply chain:

**Raw Materials Suppliers:** Employ atomistic simulations to improve understanding and predict properties of downstream products; offer optimized raw materials to compounders.

**Polymer Compounders:** Use atomistic simulations to understand formulation chemistry and predict properties; provide detailed requirements to raw materials suppliers and offer optimized products to end product manufacturers.

**End Product Manufacturers:** Leverage atomistic simulations to predict the performance of final products and quickly identify causes of failure; give specific formulation requirements to compounders.



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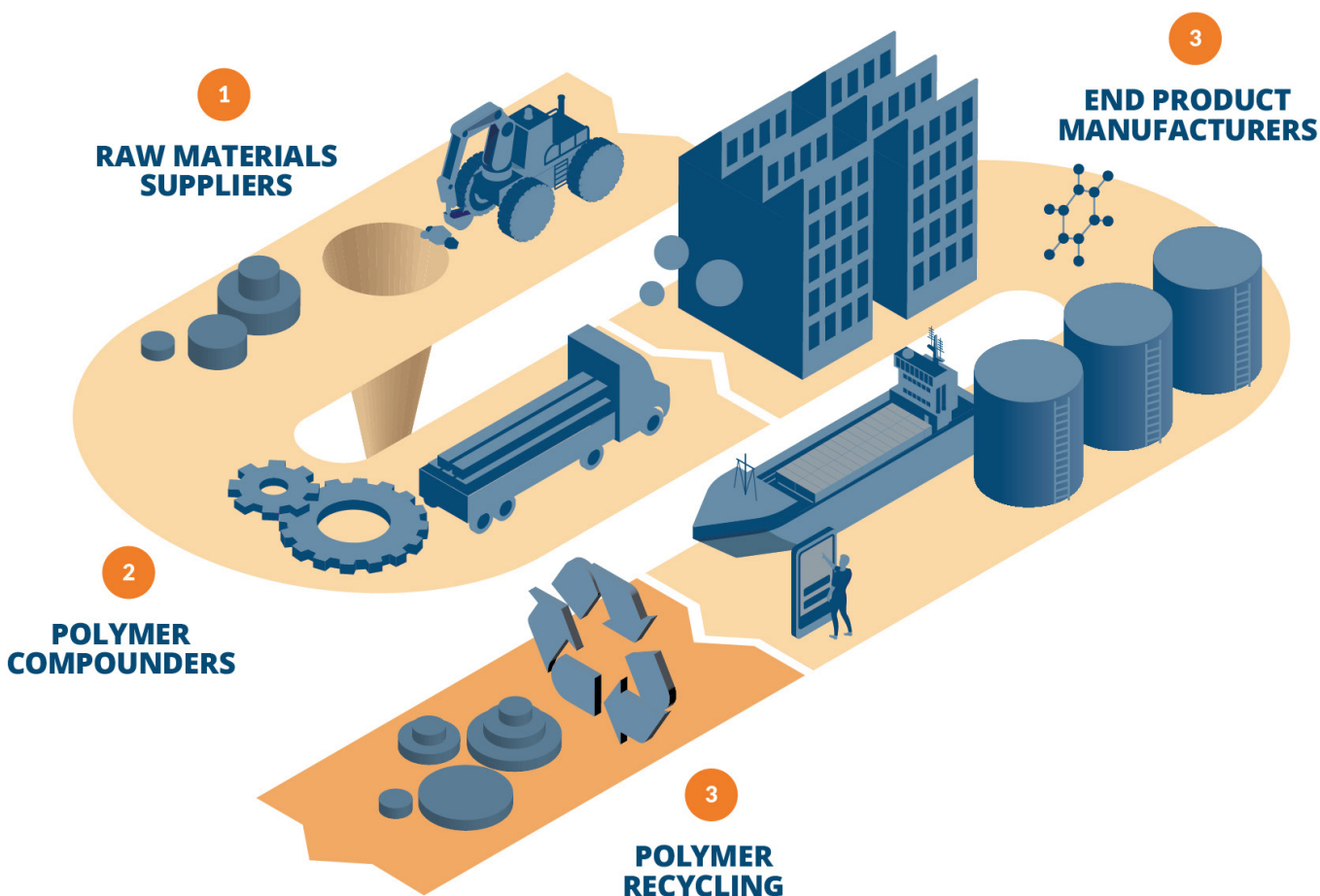
Materials

# Solution Overview

Schrödinger's Materials Science platform offers tailored solutions for research and business throughout the polymer supply chain, with differentiated model builders, efficient simulation engines accelerated by GPU computing power, automated thermophysical and mechanical response workflows, and accurate analysis tools.

- Broad molecular simulation and property prediction tools for: Thermal Properties, Mechanical and Dielectric Properties, Reactivity and Kinetics, Aggregation in Polymer Production, Solvent Sensitivity, Gas, Ion, Additive Diffusivity, Phase Morphology and SAXS Scattering, Semi-crystalline Morphology
- Applicable to all polymer types: thermoplastic homo and copolymers, crosslinked, elastomers, and dendrimers
- Intuitive user interface with automated workflows for experts or non-experts
- Dedicated scientific/technical support and vast learning resources

## Digital Chemistry Value Across Polymer Supply Chain (Example: Transportation Industry)



1

## Raw Materials Suppliers

Suppliers of petrochemical and chemical feedstocks, additives, and various monomers and resins

### Design new chemistries from alternative sources and discover new applications through simulating downstream products properties

- Predict polymer crosslinker performance in composite matrix resins such as epoxy-amine and cyanate esters
- Simulate the interaction between thermoplastic styrene-butadiene and crosslinkers

### Speed decision making for catalyst selection in raw materials production

- Simulate and understand the catalysis mechanisms, selectivity, and reactivity of epoxy amine, urethane, and other reactions

### Develop alternative greener raw materials that are more environmentally sustainable

- Simulate the impact of degradation on modulus for a chemistry of focus

2

## Polymer Compounders

Suppliers who prepare polymer formulations by mixing or/and blending polymers and additives into process-ready products

### Predict the performance of alternative raw materials in formulations and end products

- Predict glass transition, thermal stability, and thermal expansion with new polymers
- Quantify the diffusion of additive in polymers
- Understand water transport and morphological stability of polymer formulations

### Efficiently optimize formulation properties

- Predict and track water uptake in polymer composites
- Predict curing kinetics and processing properties

### Develop greener formulations that are more environmentally sustainable

- Simulate and screen for optimal formulation with new bio-based chemistry

3

## End Product Manufacturers

Processors of resins/formulations who make them into finished products on the market

### Enable reliable decision-making through predictive modeling of end product properties

- Predict tire materials performance with different additives and cross-linkers

### Obtain best chemistry from upstream suppliers by targeted chemical design to properties critical to product and processing constraints

- High-throughput screening of epoxy-amine reactions to identify the unique combinations for target properties

### Accelerate the manufacturing process pipeline

- Predict polymer gelling during manufacturing process

### Quickly screen and identify potential causes and impacts of manufacturing and material source deviations

- Predict sensitivity of matrix to cleaning solvents

### 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

4

## Polymer Recycling

Research and design for recyclability throughout the polymer supply chain

### Design polymers for recyclability

- Predict selectivity of chemical recycling reaction

### Expand use of recycled materials

- Simulate impact of recycled polymers in packaging

### Determine impact on product with use of recycled material

- Screen for property changes with recycling driven microstructure changes

# About Schrödinger

Schrödinger is transforming the way materials are discovered. Schrödinger has pioneered a physics-based software platform that enables discovery of high-quality, novel molecules for materials applications more rapidly and at lower cost compared to traditional methods.

[Learn how digital chemistry is driving innovation across materials science industries](#)

**Contact us:** [sales@schrodinger.com](mailto:sales@schrodinger.com)

**Learn more:** [www.schrodinger.com/materials-science](http://www.schrodinger.com/materials-science)

