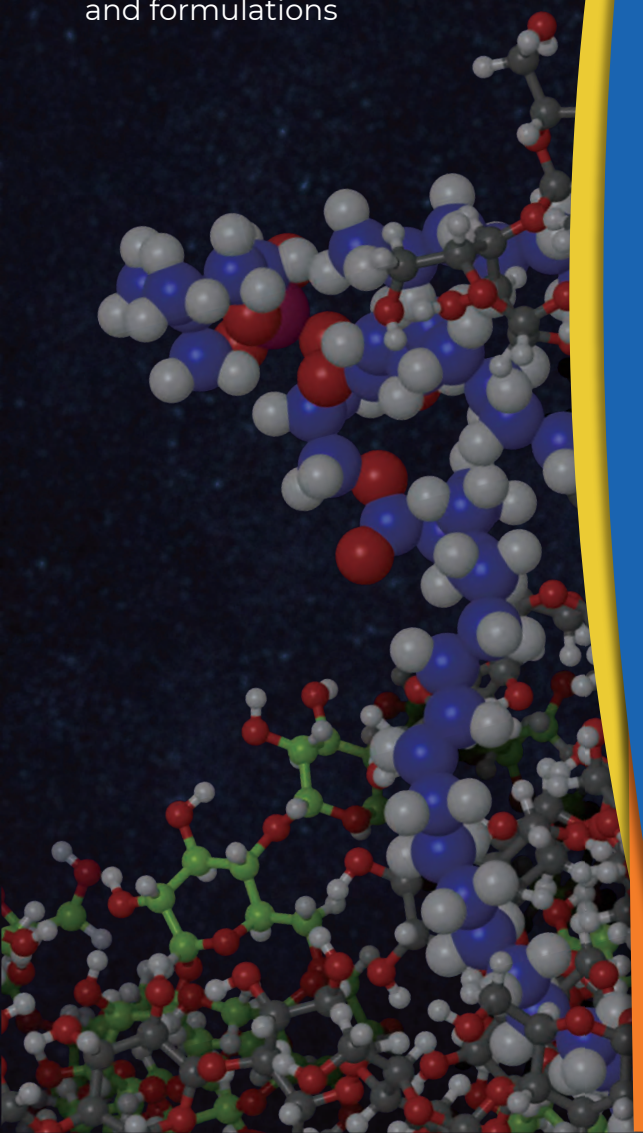
MOLECULAR SIMULATION FOR

CONSUMER PACKAGED GOODS PRODUCT DEVELOPMENT

Integrated software tools for predicting food nano-architecture, ingredient stability and safety, packaging materials, and formulations



EMPOWER COLLABORATION

- Enterprise tools for sharing experimental and predictive models seamlessly
- Rapid deployment of machine learning models to drive predictions
- Work side by side, accelerating project communication and collective learning
- Expert-level modeling: screen, share results, and make informed decisions

IDENTIFY KEY PROPERTIES

- Determine chemical properties in-silico, reducing costly experiments
- Screen libraries of FDA-approved molecules for food consumption, cosmetics, and packaging
- Rapidly build machine learning predictive models using sensory, physiochemical, and/or biological data

ACCELERATE PRODUCT DEVELOPMENT

- Drive projects forward with rapid, high-throughput prediction of materials properties
- Fill in experimental knowledge gaps of your products with simulation
- Efficiently explore chemical space of novel molecules and/or formulations

SCHRÖDINGER®

MODEL COMPLEX SURFACTANT FORMULATIONS / EMULSIONS

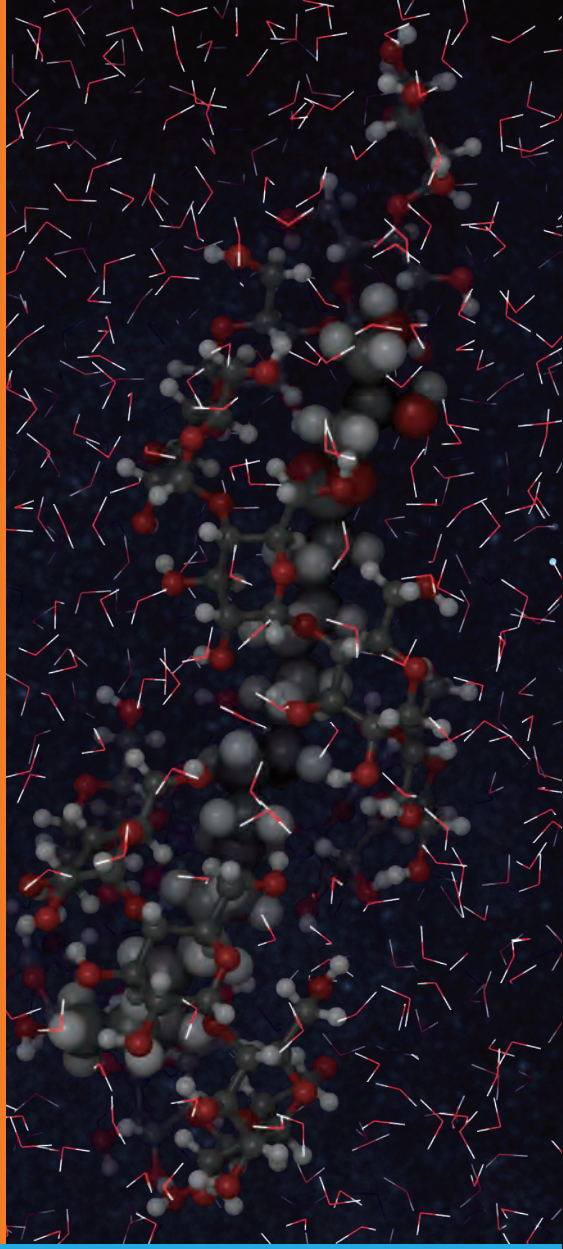
- Predict morphology of complex surfactant systems using all-atom or coarse-grained models
- Provide insight to microemulsion structure, interfacial properties, and thermodynamics not accessible with experimental methods
- Drive formulation development through virtual screening of surfactant systems

MAXIMIZE PROPERTIES OF PACKAGING MATERIALS

- Minimize production waste of packaging materials by predicting thermomechanical properties
- Innovate novel materials for active, recyclable, and bio-based materials through molecular simulation
- Rapidly investigate the ability to scale to manufacturing-level processes

PREDICTION OF PHYSI-COCHEMICAL PROPERTIES

- Predict stability, decomposition, and spectroscopic properties of molecules
- Incorporate feedback from consumers related to sensory, toxicological, and chemical properties into predictive machine learning informatics-based methods
- Build realistic models using multiple ingredients, encapsulating polymers, and additives



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