INDUSTRY APPLICATION

Application of Molecular Simulation and Machine Learning in Consumer Packaged Goods

Schrödinger offers powerful, easy to use solutions for CPG product research and development. Designed for non-expert and expert users alike, the Schrödinger platform offers simple workflows for building, simulating and analyzing real-life systems with advanced physics-based modeling and machine learning technology.

Schrödinger's team of dedicated Scientific and Technology Support experts bring domain-level expertise to ensure users gain the most project impact from the platform. Additional research services and collaboration opportunities are available.

Here we present example applications of Schrödinger's Consumer Packaged Goods capabilities.

Schrödinger | Materials

Food and Beverage

Advance food processing and bio-based packaging

Predict water uptake, transport and plasticization in starch

Extend product shelf life

Predict chemical stability and understand antifungal mechanism of edible coating

Incorporate plant based-protein ingredients

Understand aggregation and emulsifying properties and mechanism for emulsions and foam

Predict and design flavors and scents

Understand taste mechanisms with deep learning and informatics-based methods

Understand food emulsions and architecture

Predict morphology of complex emulsions

Cosmetic and Personal Care

Optimize shampoo formulations

Model and quantify interface interactions between F-layers of hair follicles and shampoo formulations

Replace traditional surfactants

Simulate micelle formation, morphology, and self assembly of emulsifier into micelles

Understand microemulsions

Explore phase diagrams, multi-component separation/aggregation of microemulsion systems

Drive formulation development

Perform virtual screening of surfactant systems

Build realistic models for complex formulations

Construct mixtures of multiple ingredients, encapsulating polymers, and additives

Cleaning Products

Improve cleaning efficiency

Understand self assembly and morphology of cleaning surfactants on surfaces and the effect of environment (e.g. temperature) on the changes of efficiency

Understand micelle formation

Predict self assembly of surfactants

Understand microemulsions

Provide insight to structure, interfacial properties, and thermodynamics

Advance formulation stability

Predict stability, decomposition, and spectroscopic properties of molecules (e.g antioxidants)

Packaging

Develop sustainable packaging

Study interfacial interactions between packaging materials and consumer goods, and simulate water uptake for barrier design and performance

Minimize production waste

Predict thermomechanical properties of packaging materials

Innovate with natural materials

Explore active, recyclable, and bio-based materials through molecular simulation

Reduce processing cost

Investigate the ability to scale to manufacturing-level processes

Team Collaboration and Digital Data Management

Empower collaboration

Employ enterprise informatics tools for sharing experimental and predictive models seamlessly

Amplify research

Rapid deployment of machine learning models to drive predictions

Promote project management

Work side by side, accelerating project communication and collective learning; screen, share results, and make informed decisions

Products

Check on the products that enable your success in the CPG industry.
Download our Materials Science Product Guide.

Desmond

Highly efficient Molecular Dynamics (MD) tool

- MD multi-stage workflow
- Free energy calculation (FEP+ solubility, metadynamics, replica exchange)
- Simulated annealing

AutoQSAR

Automated machine learning tool

- 1D, 2D and 3D descriptor builder
- Model building and auto-selection
- Make prediction

MS CG

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

- Coarse-grained sketcher
- Coarse-grained force fields: Dissipative particle dynamics, Martini, Generalized Lennard-Jones + Coulomb

MS LiveDesign

Web-based enterprise informatics for materials design

- Digital data management
- Team collaborations across geographies and organizations

OPLS4

Advanced modern force field

- Force field builder
- Conformational analysis

MS Jaguar

Rapid ab initio electronic structure package

- Bond and ligand dissociation
- Reaction analysis
- Charge transport

Selected Publications

Molecular-Level Examination of Amorphous Solid Dispersion Dissolution
Mohammad Atif Faiz Afzal, Kristin Lehmkemper, Ekaterina Sobich, Thomas F. Hughes, David J. Giesen, Teng Zhang, Caroline M. Krauter, Paul Winget, Matthias Degenhardt, Samuel O. Kyerematenge*, Andrea R. Browning, and John C. Shelley*
Mol. Pharmaceutics 2021, 18, 11, 3999-4014

The structural basis of odorant recognition in insect olfactory receptors
Josefina del Mármol, Mackenzie A. Yedlin & Vanessa Ruta
Nature 2021, 597, 126-131

Characterizing moisture uptake and plasticization effects of water on amorphous amylose starch models using molecular dynamics methods
Jeffrey M.Sanders, Mayank Misra, Thomas J.L.Mustard, David J.Giesen, Teng Zhang, John Shelley, Mathew D.Halls
Carbohydrate Polymers 2021, 252, 11716

Comprehensive structure-activity-relationship studies of sensory active compounds in licorice (Glycyrrhiza glabra)
Christian Schmid, Anne Brockhoff, Yaron Ben Shoshan-Galeczki, Maximilian Kranz, Timo D. Stark, Rukiye Erkaya, Wolfgang Meyerhof, Masha Y. Niv, Corinna Dawid, Thomas Hofmann
Food Chemistry 2021, 364, 130420

In Silico Investigation of Bitter Hop-Derived Compounds and Their Cognate Bitter Taste Receptors
Andreas Dunkel, Thomas Hofmann, and Antonella Di Pizio
J. Agric. Food Chem. 2020, 68, 38, 10414-10423

Structure-based screening for discovery of sweet compounds
Yaron Ben Shoshan-Galeczki, Masha Y Niv
Food Chemistry 2020, 315, 126286

Bitter or not? BitterPredict, a tool for predicting taste from chemical structure
Dagan-Wiener, A.; Nissim, I.; Ben Abu, N.; Borgonovo, G.; Bassoli, A.; Niv, M.Y.
Scientific Reports 2017, 7, 12074

Molecular Dynamics Simulation Study of Sodium Dodecyl Sulfate Micelle: Water Penetration and Sodium Dodecyl Sulfate Dissociation
Chun, B.J.; Choi, J.I.; Jang, S.S.
Colloids and Surfaces A: Physicochemical and Engineering Aspects 2015, 474, 36

Contact us: sales@schrodinger.com
Learn more: www.schrodinger.com/materials-science

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