MATERIALS SCIENCE

Contract Research Services

Leverage Schrödinger's scientific and engineering expertise

Apply advanced simulation tools to solve your materials science research challenges

Free up time and resources

Let our scientists execute the project while collaborating closely with your team

Data security is of utmost importance

Contract research customers retain all intellectual property

Best suited for companies and teams who want to:

- Reduce time spent on trial-and-error experiments
- Leverage Schrödinger's advanced physics-based and machine learning methods and expertise
- Gain molecular-level insight into their materials
- Explore the benefits of digital approaches before investing in in-house adoption

Schrödinger's industry-leading technologies

- Quantum mechanics modeling
- Molecular dynamics simulation
- Molecular mechanics
- Advanced AI/ML/Active Learning/ De novo design
- Machine learning force fields (MLFFs)

Schrödinger

Advance your materials R&D with unrivaled technologies and expertise

Benefit from the full impact of Schrödinger technologies at scale

Services include all computing, licensing, and service hours required to perform comprehensive simulation projects tailored to your R&D needs.

Leverage flexible, customized solutions to ensure project success

No internal software, hardware, or computational resources needed. Benefit from expert knowledge transfer and training throughout and beyond the project. Get tailored tools and solutions designed specifically to meet your project goals.

Complement your domain expert knowledge with our expertise

After collaborating to scope out a work product, dedicated Schrödinger experts in both materials applications and digital simulations execute your projects.

Proven success

Customers across industries have trusted us with their research needs.

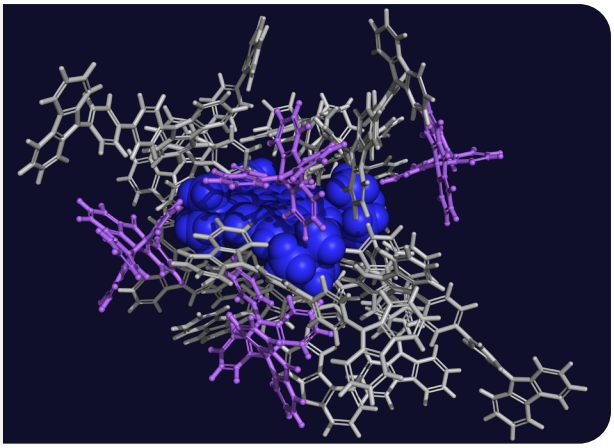
Panasonic INDUSTRY · BRIDGESTONE · SAMSUNG · reckitt · KONICA MINOLTA

L'ORÉAL · EVONIK Leading Beyond Chemistry · abbvie · سابك sabic

Example prediction capabilities by application

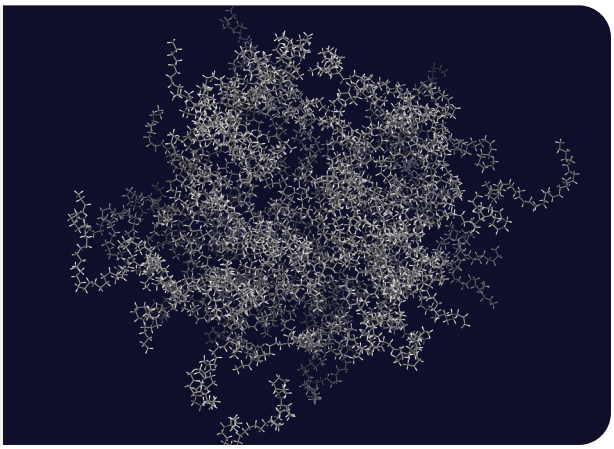
Organic Electronics

Optoelectronic properties such as photoluminescence spectra, charge transport and recombination behaviors, outcoupling efficiency, and various molecular electronic film properties



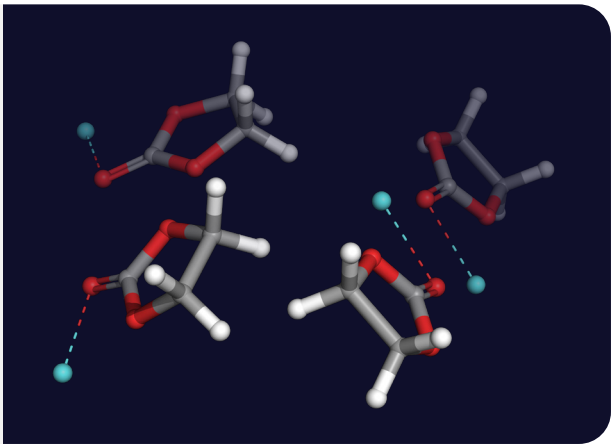
Polymeric Materials

Key physicochemical and processing properties, such as glass transition temperature (T_g), coefficient of thermal expansion (CTE), mechanical response, water uptake, cure shrinkage, diffusivity and migration as well as critical indicators of adverse environmental effects such as degradation



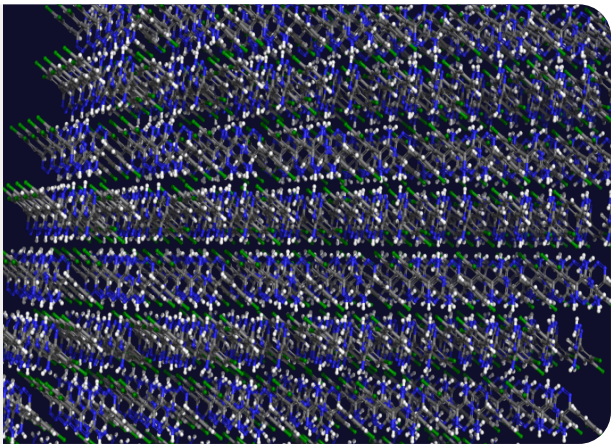
Energy Capture & Storage

Structural and transport properties of battery electrodes and electrolytes, interfacial reactivity and morphological characteristics of solid electrolyte interphases (SEI) for energy storage applications



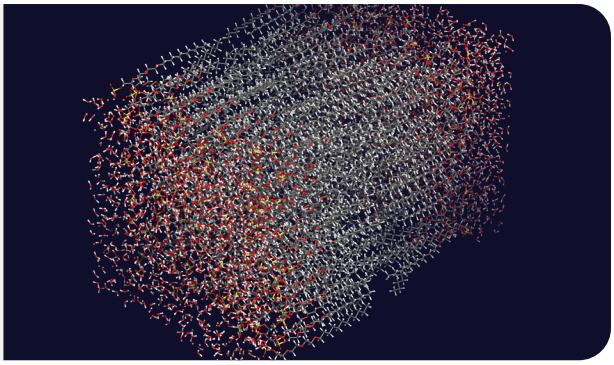
Pharmaceutical Formulations

Crystalline or amorphous form characterization, catalysis and reactivity, spectroscopy, crystal structure prediction, and formulation and delivery



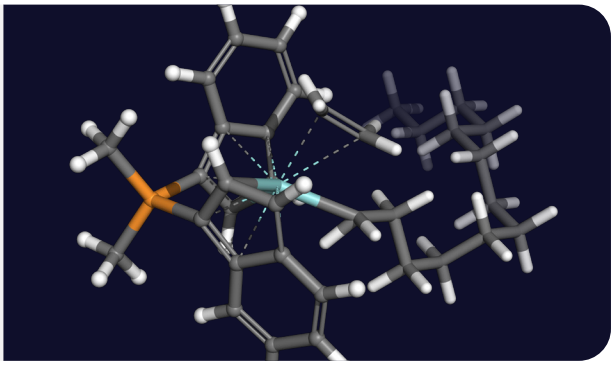
Consumer Packaged Goods

Key properties across food, cosmetics, and packaging — from ingredients to complex formulations — including phase behavior, transport properties, formulation compatibility, and sensory attributes such as texture and flavor release



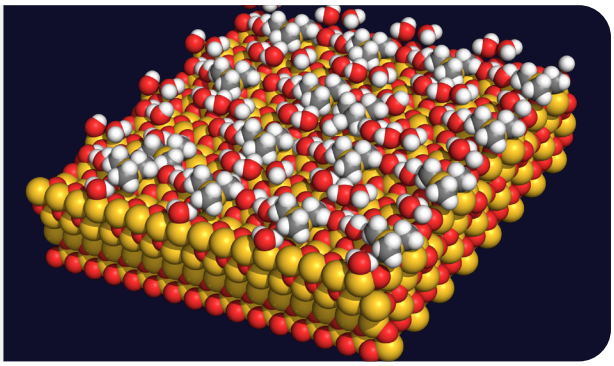
Catalysis & Reactivity

Supervised and unsupervised mechanism discovery, automated transition state search, reaction and reactivity optimization, molecular catalyst design



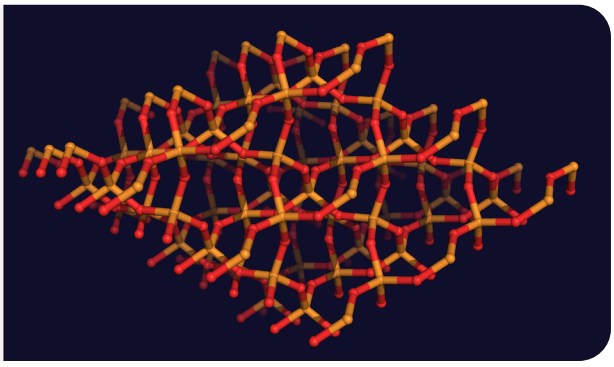
Thin Film Processing

Precursor properties (e.g. volatility, thermal stability) and gas-surface chemistry for thin film deposition or etch processes in the semiconductor industry



Metals, Alloys & Ceramics

Mechanical strength, dielectric properties, surface and interface structures, and spectral characteristics of ceramic and metallic solids



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