

# MATERIALS DESIGN AND SIMULATION

Integrated software solutions for  
atomic-scale simulation of  
chemical systems

## ACCELERATE YOUR RESEARCH

- Make decisions more confidently through the scientific accuracy of Schrödinger's proven methodologies
- Extend your knowledge base by leveraging the experience of over 200 PhD research scientists at Schrödinger with expertise across computational research areas
- Stay up-to-date with the latest scientific advances with quarterly updates

## STREAMLINE EFFORTS ACROSS THE ENTIRE PROJECT TEAM

- Put the power of modeling in the hands of your entire project team from scientist to project manager
- Facilitate ideation and communication at key phases in the materials discovery process
- Capture, share, and analyze your experimental and computational results all in one place

## SPEED-UP DEVELOPMENT TIMELINES

- Drive projects forward with cutting-edge automation, practical applications of machine-learning, and GPU-enabled computational power
- Virtually screen massive libraries of compounds

SCHRÖDINGER®



## ADVANCED MATERIALS AND PROCESS SIMULATIONS

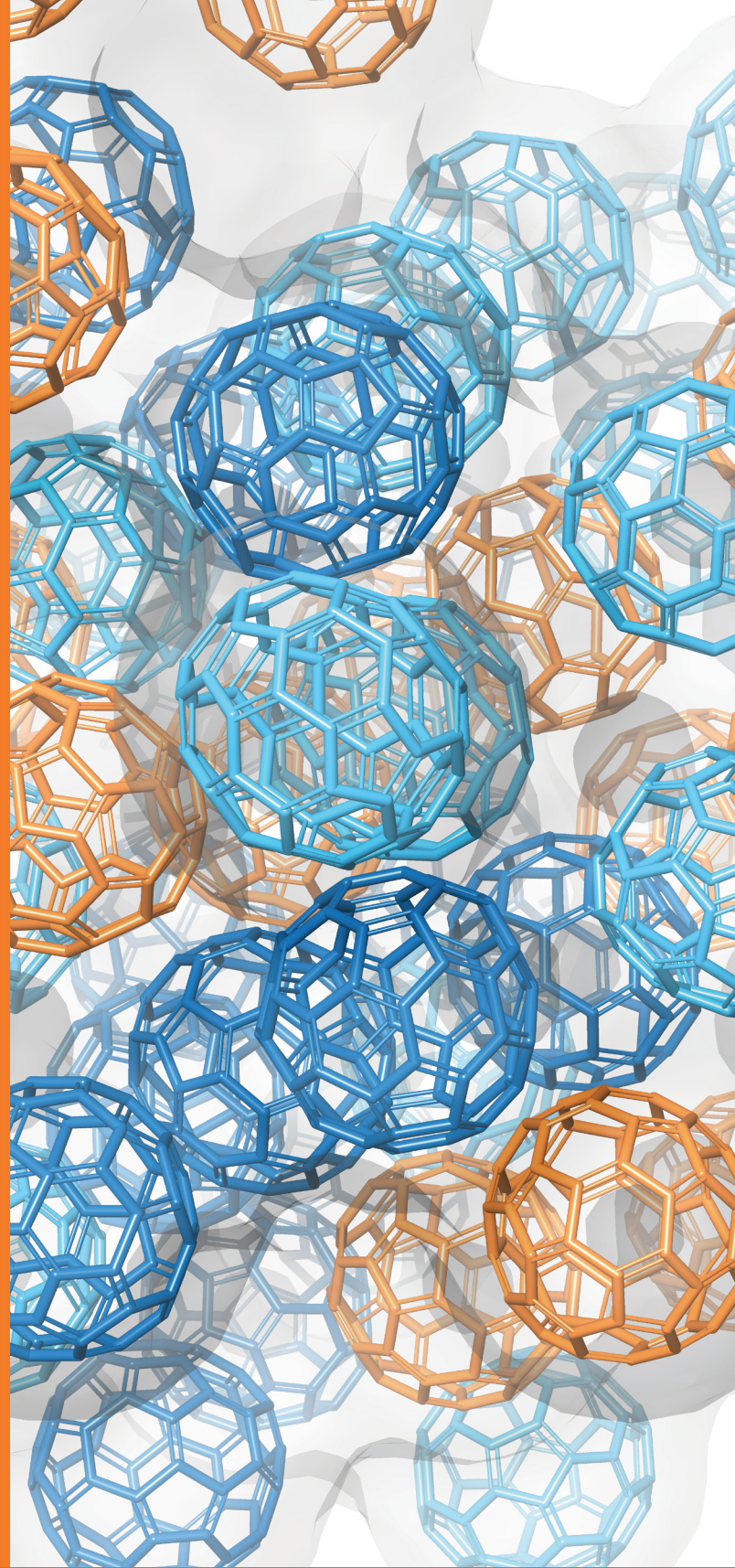
- Create models by 2D sketcher, interactive 3D building, and specialized builders
- Quantum chemical calculations for ground and excited states
- Classical simulations for discrete or periodic systems
- Integrated plotting, visual data mining, and filtering

## ATOMISTIC MODEL BUILDERS AND PROPERTY WORKFLOWS

- Specialized builders for a diverse range of systems
- Automated workflows for numerous properties including optoelectronics, electrochemistry, thermophysical properties, and more

## AUTOMATED DISCOVERY AND OPTIMIZATION

- Deterministic virtual screening through facile library generation and highly efficient automated property evaluation
- Structural enumeration: R-group, elemental enumeration, organometallics, polymer composition, and disordered systems



## FIND THE SOLUTIONS YOU'RE LOOKING FOR:



### DRUG DISCOVERY

Comprehensive solutions, validated across hundreds of targets, to accelerate lead discovery and optimization.

### MATERIALS SCIENCE

Integrated solutions for atomic-scale simulation of chemical systems to design novel polymers and other products essential to modern life.

### ENTERPRISE INFORMATICS WITH LIVEDESIGN

Breaks down traditional silo walls to unleash the power of real-time collaborative design and project management.

**REQUEST A  
FREE TRIAL**



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