Materials Science Product Guide

Discover a digital chemistry platform governed by physics-based modeling, amplified by machine learning/AI and optimized through team-based intelligence.

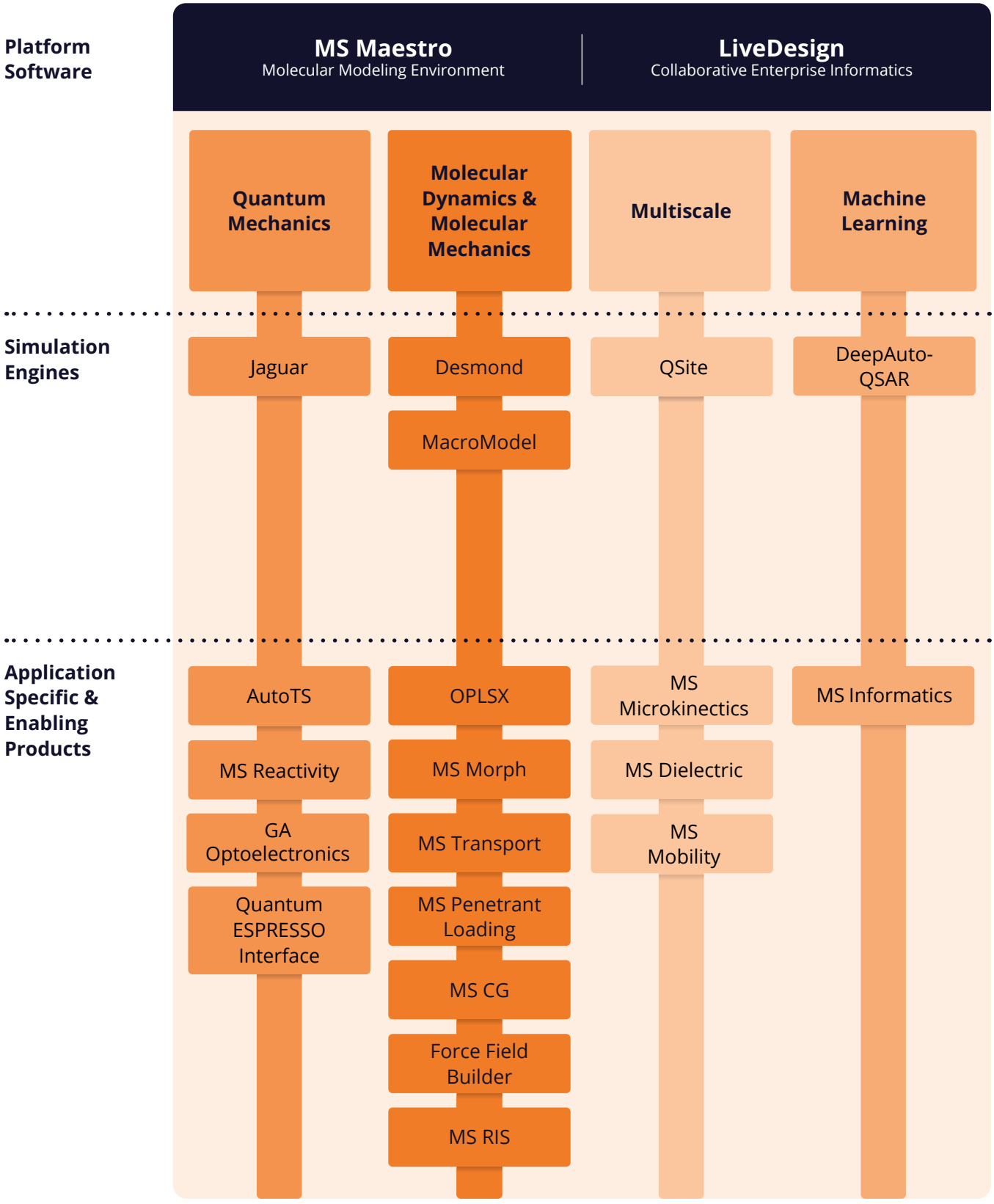
Schrödinger | Materials

Applications

Schrödinger's Materials Science solutions offer molecular-level insight into the mechanisms and properties of chemistry and materials across a wide range of applications:

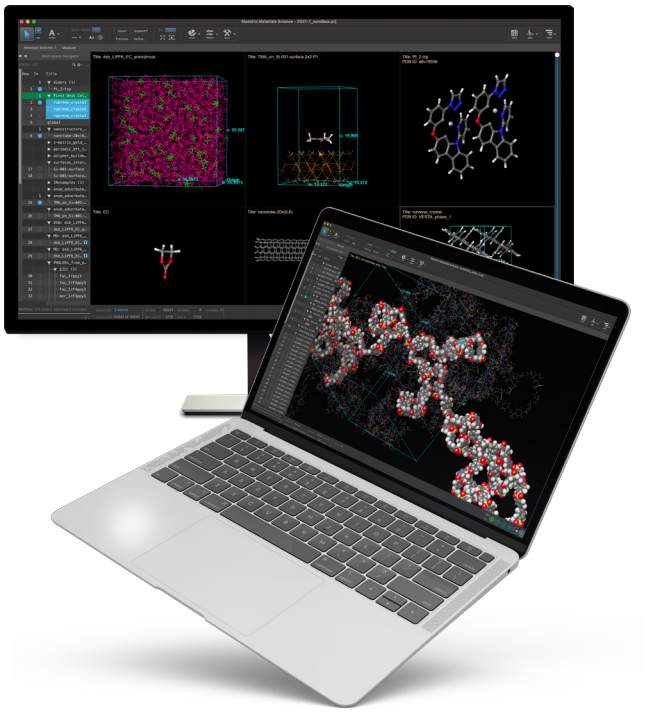
- Organic Electronics
- Polymeric Materials
- Consumer Packaged Goods
- Catalysis & Reactivity
- Thin Film Processing
- Energy Capture & Storage
- Pharmaceutical Formulations & Delivery
- Metals, Alloys & Ceramics

Product Overview



MS Maestro

MS Maestro is a streamlined interface for structural visualization, cutting-edge predictive computational modeling and machine learning workflows for materials science discovery and analysis. MS Maestro enables users at all levels of experience to work efficiently and produce impactful results.



Capabilities

- Accesses various automated simulations powered by quantum mechanics (QM), molecular dynamics (MD), and molecular mechanics (MM) through a single, unified and integrated modeling environment
- Builds realistic structural models of molecules, crystals, organometallic complexes, polymers, slabs and interfaces, and more with advanced structure builders
- Accesses advanced machine learning and cheminformatics solutions for predictive model building and validation
- Offers out-of-the-box combinatorial chemistry solutions including structural enumeration for automated library generation
- Includes comprehensive data analysis tools to use computation outputs to guide decision-making
- Enables three-dimensional visualization and manipulation of input and output structures from various modeling tasks
- Manages large-scale computational modeling and simulation tasks on local or remote compute servers across Linux, Windows, Mac and cloud

LiveDesign

LiveDesign is a powerful web-based informatics and molecular design platform that enables teams to rapidly advance materials discovery projects by collaborating, designing, experimenting, analyzing, tracking, and reporting in a centralized platform. This collaborative ideation solution enables teams of computational, synthetic, analytical, process scientists, and engineers to work through problems and share results on a unified platform.

Capabilities

- Deploys powerful computational models widely within organizations, democratizing predictive models for computational chemists, experimentalists, collaborators and leadership
- Shares live computational and experimental data and design ideas for rapid decision making
- Leverages machine learning capabilities for continuous model refinement based on the latest available data, and extends to customized de novo design
- Integrates cheminformatics and data sharing for collaboration across organizations and geographic locations
- Facilitates project management and analytics, accelerates project communication, and ensures collective learning

Quantum Mechanics

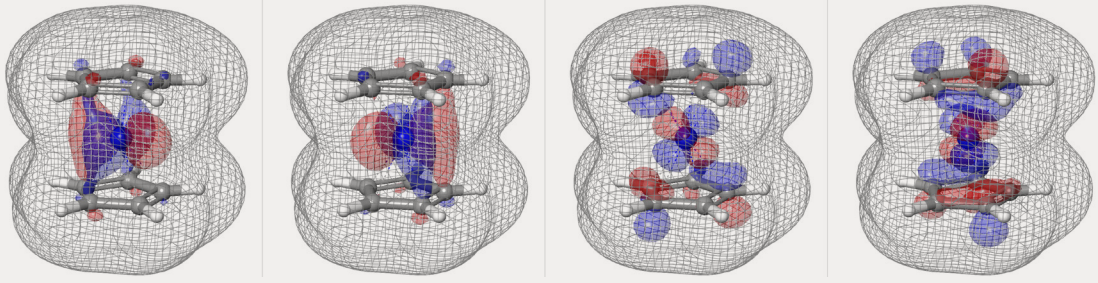
Jaguar

Jaguar is a well-validated, robust, high-performance quantum mechanics package that specializes in fast predictions of electronic structure and properties for molecular systems of all sizes via the use of pseudospectral density functional theory (PS-DFT) based method which scales favorably with system size. Jaguar can also be used for the ab initio-assisted design and high throughput virtual screening of new materials solutions with novel or enhanced properties for a variety of applications such as catalysts, batteries, organic electronics, and more.

Capabilities

- Offers a wide range of types of molecular QM calculations: geometry optimization, transition state search, thermochemical properties, implicit solvation, spectra prediction, etc.
- Integrated with xTB for semi-empirical calculations and QRNN for machine learned potentials
- Supports a wide variety of DFT functionals with analytic second derivatives and dispersion corrections
- Offers sophisticated geometry constraints, including rigid and relaxed scans
- Performs relativistic DFT calculations
- Provides several times speedup at a negligible accuracy loss with optional pseudospectral approximation
- Offers a range of automated solutions, e.g. pKa prediction, conformationally averaged VCD and ECD spectroscopy, tautomer generation and ranking, heat of formation, etc.
- Generates publication-quality 3D surfaces: molecular orbitals, electrostatic potential projected on isodensity, non-covalent interactions, etc.

Ferrocene $Fe(C_5H_5)_2$



HOMO-1 | HIGHEST OCCUPIED MOLECULAR ORBITAL (HOMO) | LOWEST UNOCCUPIED MOLECULAR ORBITAL (LUMO) | LUMO+1

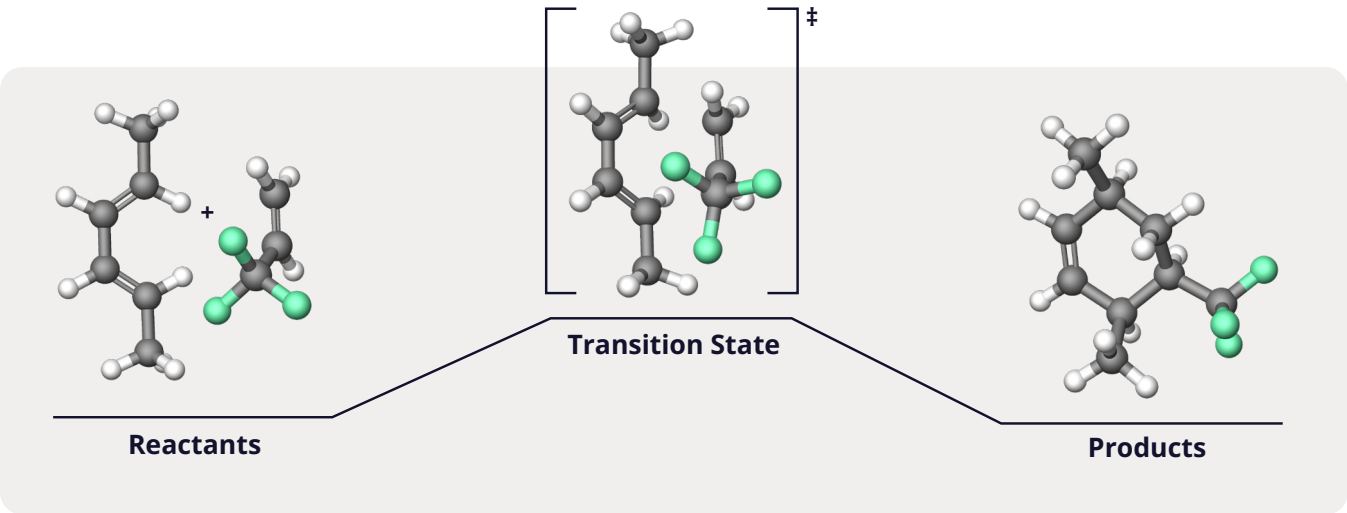
AutoTS

Transition states are essential in many materials science applications: predicting reactivity, understanding reaction mechanisms, designing and optimizing catalysts, predicting outcomes of various competing reactions, and more. Locating a transition state (TS) is necessary for computing the activation energy of a reaction, and thereby the reaction rate, and it is unique to computation. AutoTS is an automated workflow to find transition states, particularly for elementary, molecular reactions. AutoTS requires only the structures of the reactants and the products as input, and then automates the search process to obtain the transition state and the reaction energetics.

Capabilities

- Locates a TS between the reactant and product molecules with an automated solution
- Optimizes reactants and products, determines breaking and forming bonds, establishes correspondence between atoms in the reactants and the products, and generates a transition state guess
- Prints the potential energy surface diagram showing the transition state barrier
- Performs iterative transition state search finding intermediates that connect reactants and products
- Allows for frozen atoms and formally spectator reactants (like catalytic solvent molecules)
- Performs conformational search on reactants, products, and transition states, outputting statistically averaged energetics

Associated Products: Jaguar, MacroModel



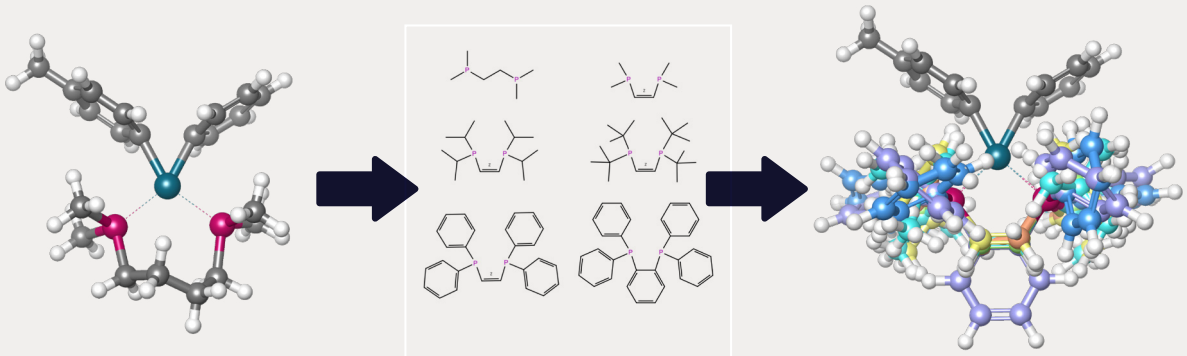
MS Reactivity

MS Reactivity offers two highly automated modules for modeling in molecular chemistry and catalysis. The first module, Automated Reaction Workflow (AutoRXNWF), is intended for chemical reaction and reactivity optimization with quantum mechanics based on a user-defined library and a reference reaction. One example of the application of AutoRXNWF is molecular catalyst design. The second module, Nanoreactor, is intended to identify reaction products for any reaction and sort them based on thermodynamics principles. This is achieved via automated potential energy surface (PES) sampling with semiempirical metadynamics, PES refinement, and sorting based on free energies. One of the applications of Nanoreactor is the study of small molecule degradation products without any prior knowledge.

Capabilities

- Automatically screens high-throughput reactions and catalysts for prediction of reactivity and selectivity, including free energy and solvation corrections
- Computes rates, barriers, and machine learning descriptors automatically during post processing
- Identifies lowest energy starting structures with conformational sampling
- Optimizes geometries and energies quantum mechanically with Jaguar
- Removes structures with unwanted frequencies from post processing
- Performs anharmonic correction to thermophysical properties
- Visualizes reaction coordinate images with relative energies for all properties
- Visualizes contour plots of buried volumes for catalysts
- Predicts plausible degradation products with xTB metadynamics

Associated Products: Jaguar, MacroModel



Reaction Transition State **Ligand Library** **Enumerated Reactions**

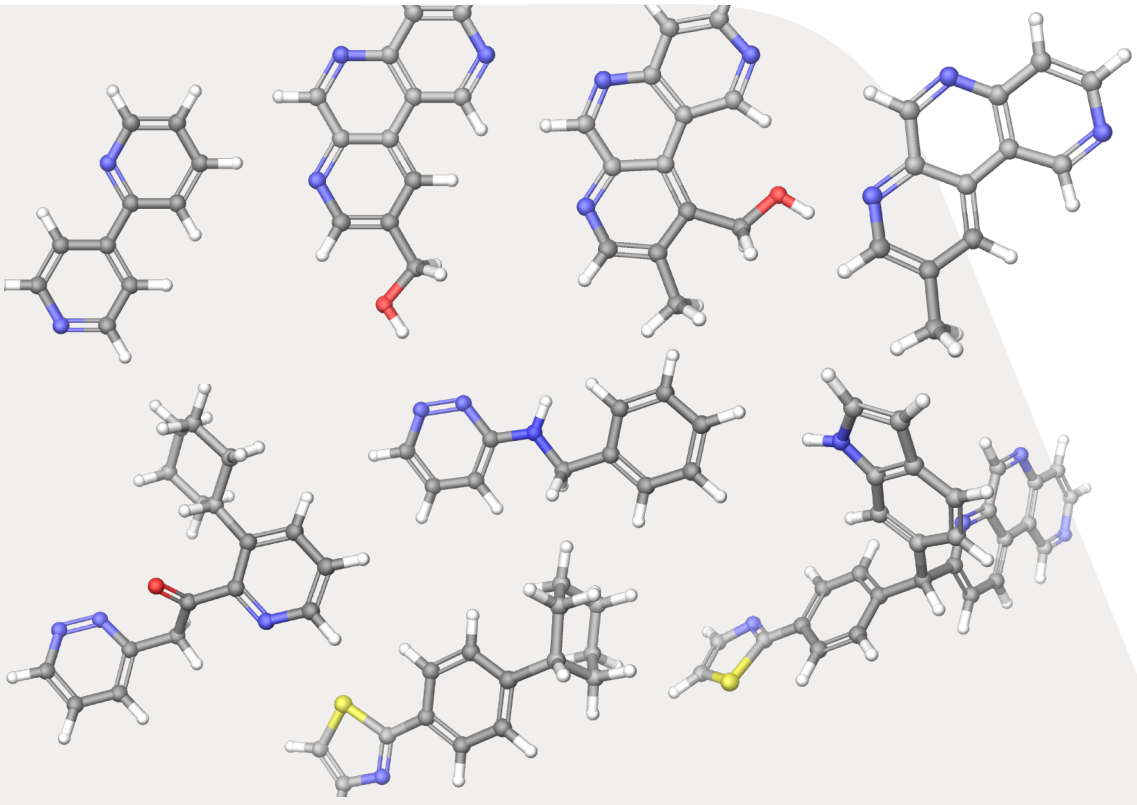
GA Optoelectronics

GA Optoelectronics enables the generation of novel chemical space for molecular materials with desired properties for optoelectronic applications via a genetic algorithm. The optoelectronics capabilities are designed to leverage rapid screening to complement experimental development by elucidating molecular properties and informing future synthetic targets.

Capabilities

- Generates a library of compounds within a target property space with genetic optimization
- Supports optimization by QM (DFT) calculated properties or by model-predicted properties via machine learning
- Supports basic molecular design constraints (number of elements, molecular weight, etc.)

Associated Product: Jaguar

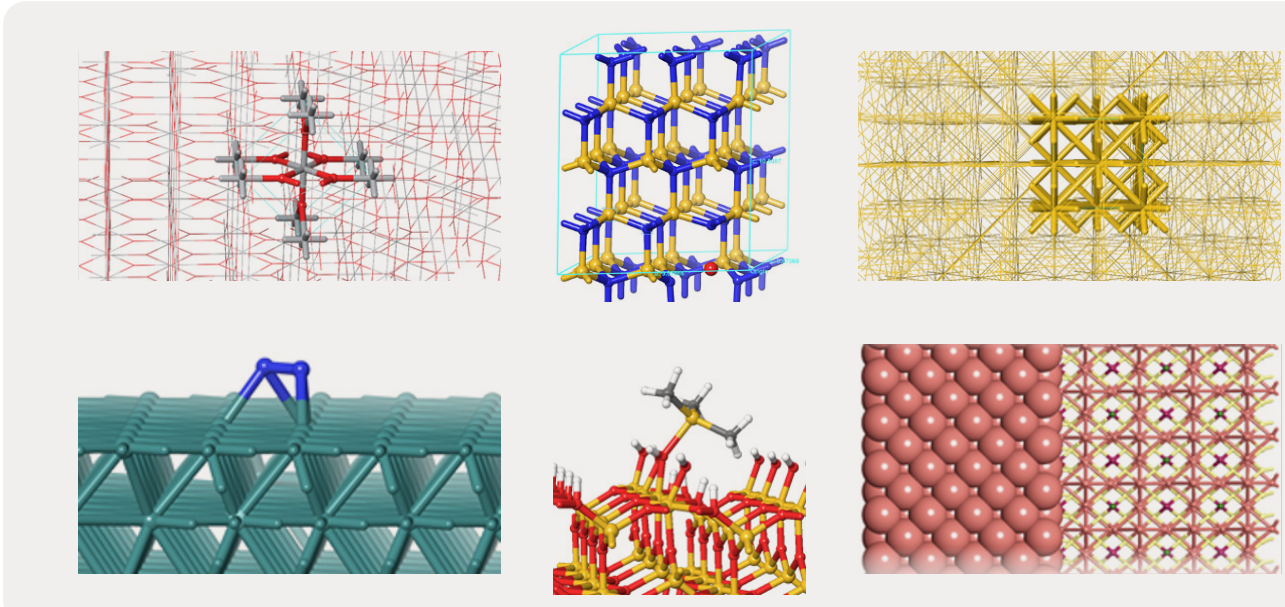


Quantum ESPRESSO Interface

Quantum ESPRESSO, developed by Quantum ESPRESSO Foundation (QEF), is the leading high-performance, open-source quantum mechanical software package for nanoscale modeling of materials. Quantum ESPRESSO implements plane wave density-functional theory in conjunction with periodic boundary conditions and pseudopotentials. Schrödinger collaborates with QEF in methods development and develops the proprietary Quantum ESPRESSO interface automating complex workflows for structure generation, calculations, and analysis. The QE interface provides a comprehensive graphical user interface for streamlined calculation set-up, job control, and results analysis, enabling ab initio modeling of bulk materials, their surfaces, and interfaces. The tool is embedded directly into MS Maestro to provide a simple user interface.

Capabilities

- Provides predictions for bulk, surface and interface properties
- Supports Ultrasoft (US), Norm-Conserving (NC) and Projector Augmented Wave (PAW) pseudopotentials
- Performs structural optimization, polymorphism and ab initio molecular dynamics
- Simulates transition states and minimum energy paths using nudged elastic band (NEB) method
- Models linear response properties within Density Functional Perturbation theory (DFPT)
- Predicts spectroscopic properties
- Predicts band structure and band gap, charge density and density differences, phonons and free energy, dielectric permittivity, and more solid-state properties



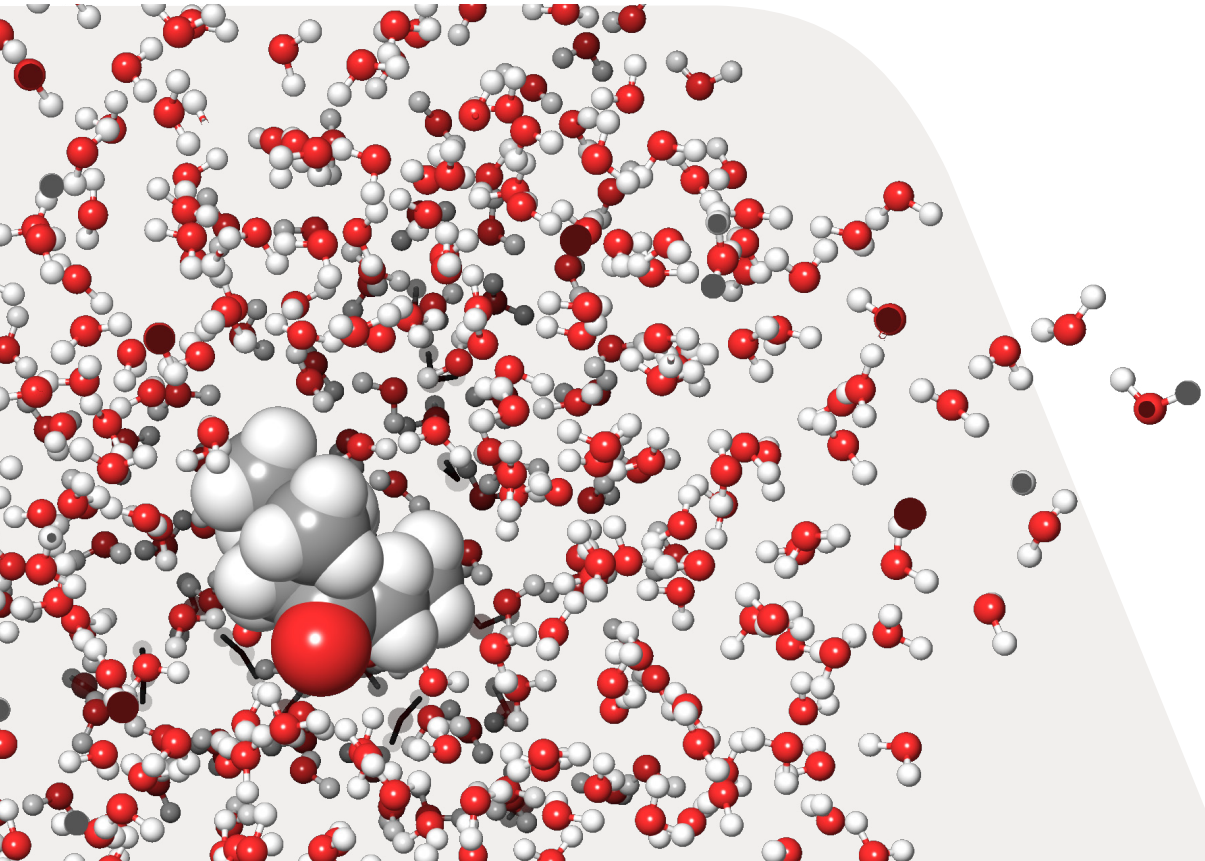
Molecular Dynamics & Molecular Mechanics

Desmond

Desmond is a GPU-powered, high-performance molecular dynamics (MD) engine providing high scalability, simulation throughput, and scientific accuracy. Desmond can be employed for predicting bulk properties of materials, such as thermophysical properties, elastic constants, stress/strain relationships, diffusion coefficients, viscosity, persistence length, free energy of solvation, and more. Desmond also characterizes structure and properties in complex systems involving non-equilibrium systems as well as interfaces or self-assembled structures.

Capabilities

- Improves computing speed by 100x on general-purpose GPU (GPGPU) versus single CPU
- Simulates single components, mixtures, and solutions with periodic boundary conditions using cubic, orthorhombic, truncated octahedron, rhombic dodecahedron, and arbitrary triclinic simulation boxes
- Simulates large scale features of nanometers to micron size over time scales of picoseconds to microseconds
- Performs accurate checkpointing for continuing or restoring simulations
- Calculates electrostatic interactions with high accuracy
- Offers simulation techniques for improved sampling, including replica exchange, metadynamics, and simulated annealing
- Supports coarse-grained force fields (with MS CG), applying all Desmond capabilities to coarse-grained modeling

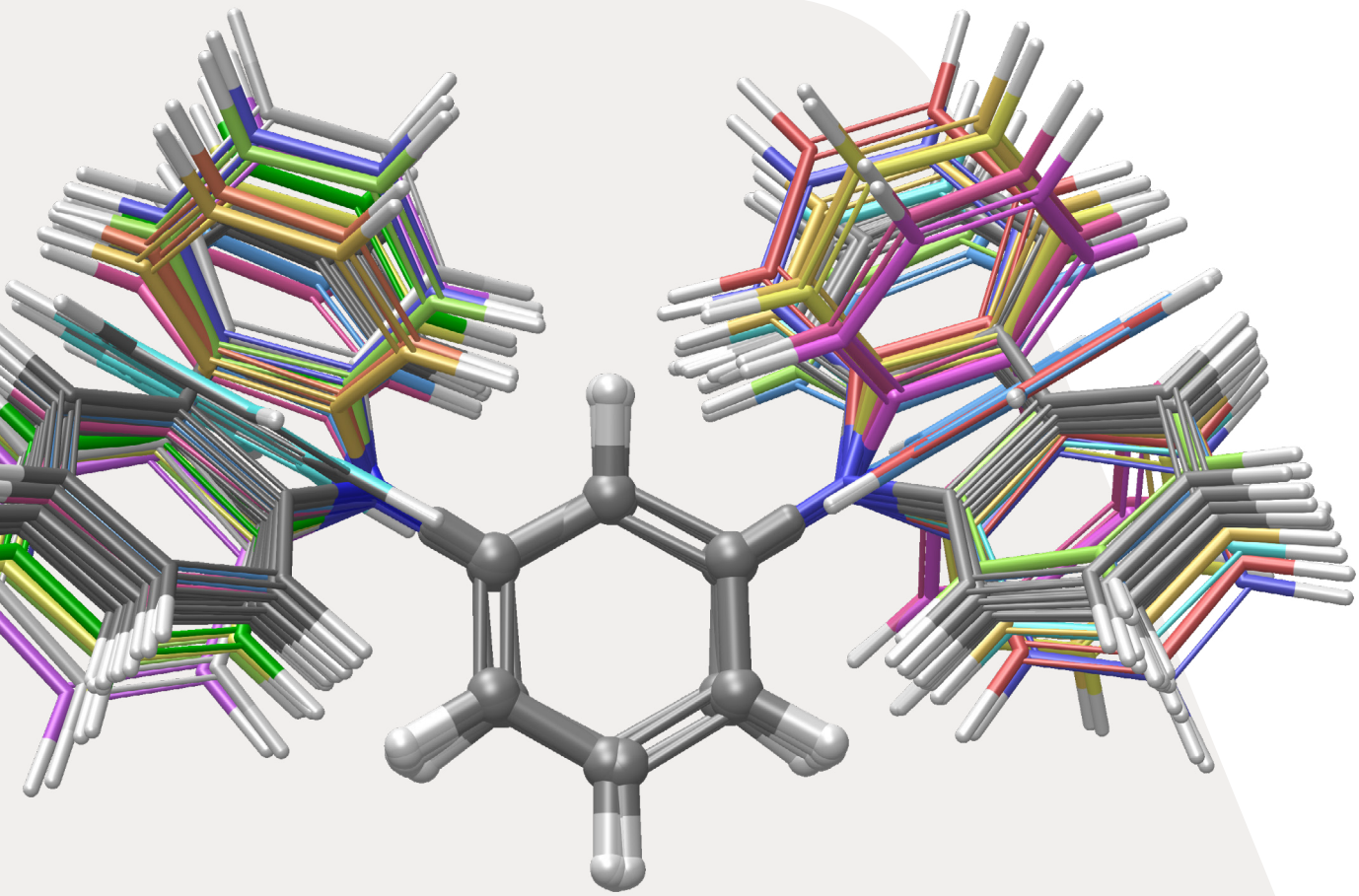


MacroModel

MacroModel is a force field-based molecular modeling tool with a range of advanced features and methods for examining molecular conformations, molecular motion, and intermolecular interactions. This flexible program can be utilized for diverse research applications, including organic and inorganic molecules and oligomers, organometallic complexes, and complex biological systems.

Capabilities

- Molecular mechanics engine for energy minimization and conformational sampling of molecular compounds
- Supports various force fields, e.g. MM2, MM3, AMBER, AMBER94, MMFF, MMFFs, OPLS-X

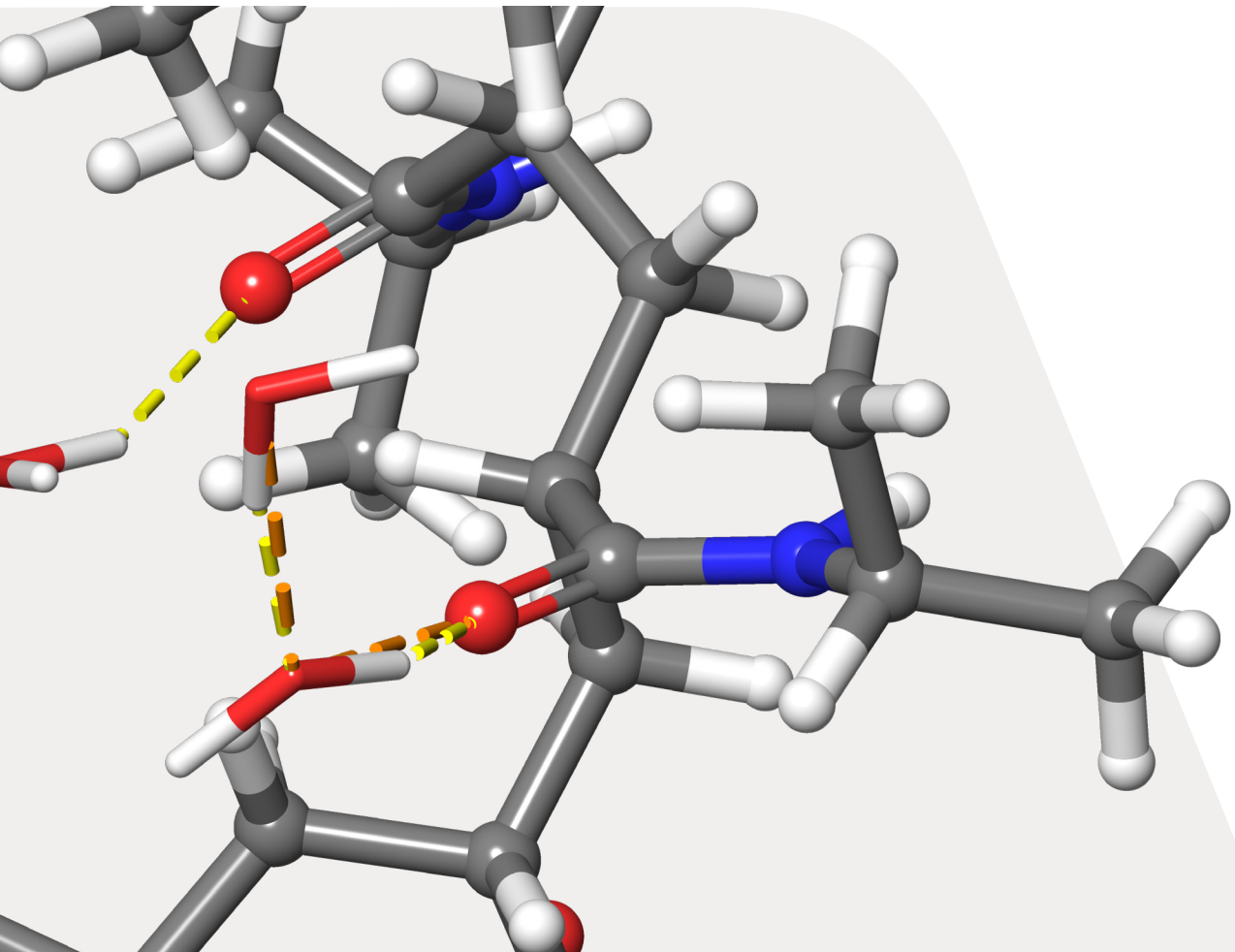


OPLS–Force Field

Accurate force field parameters are at the heart of obtaining useful molecular structures and relative energies for practical use in material design and developments. OPLS-X is Schrödinger's modern force field with consistently enhanced new versions. It offers proven performance for small molecules, organics, polymers, OLEDs, silicates, and more, providing coverage for numerous industries. OPLS provides leading accuracy through detailed parameterization.

Capabilities

- Offers commercial-grade force field for classical molecular dynamics and organic materials design
- Contains small molecule torsion parameter coverage of 95% for relevant chemical space
- Offers over 100,000 torsion types covering a wide range of chemistries and, with the addition of Force Field Builder, can create new or unique chemistry automatically
- Calculates heterocyclics and halogen off-site electron density
- Supports Desmond, MacroModel and associated application modules



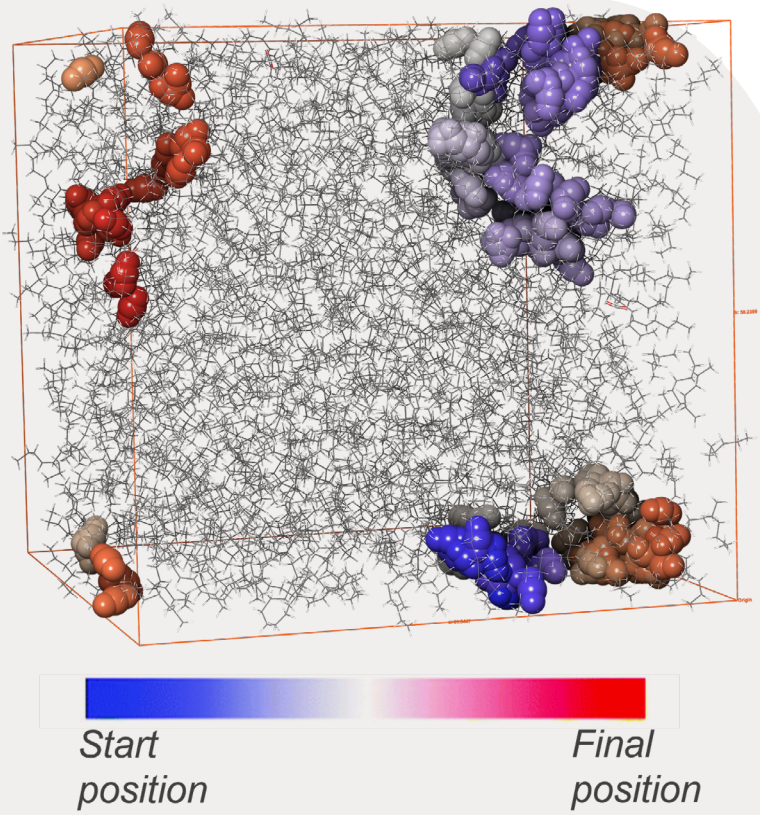
MS Transport

MS Transport provides access to molecular dynamics (MD) simulation workflows for calculating shear viscosity and the isotropic and anisotropic diffusion coefficients for a particular type of atom or molecule. From the diffusion of Li+ ions in battery polymers to the viscosity of solvents, the equilibrium MD based workflows in MS Transport provide valuable insight into the performance of materials.

Capabilities

- Leverages fast molecular dynamics simulation with Desmond to calculate diffusion and viscosity in industrially relevant wall times
- Calculates diffusion of gasses through matrices, ions through battery polymers, and additives in plastics with out-of-the-box input and viewer interfaces
- Predicts viscosity with the latest equilibrium molecular dynamics approaches
- Calculates transport properties at desired temperatures and explores the temperature dependence of diffusion and viscosity
- Visualizes diffusion and viscosity output plots

Associated Product: Desmond



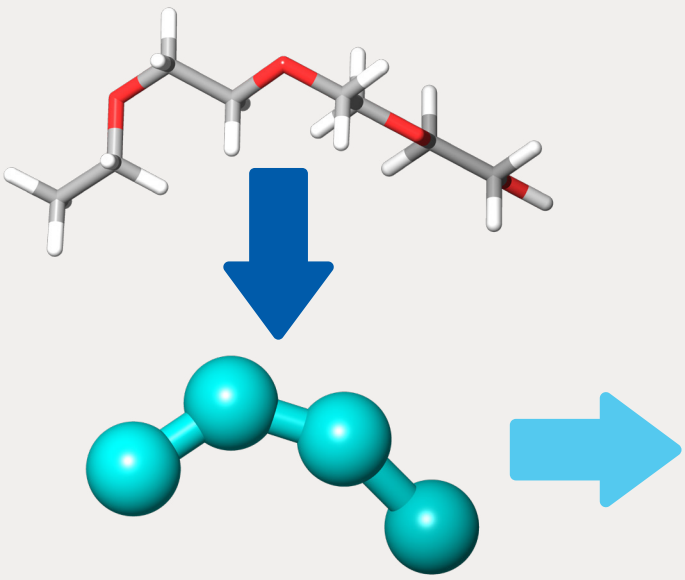
MS CG

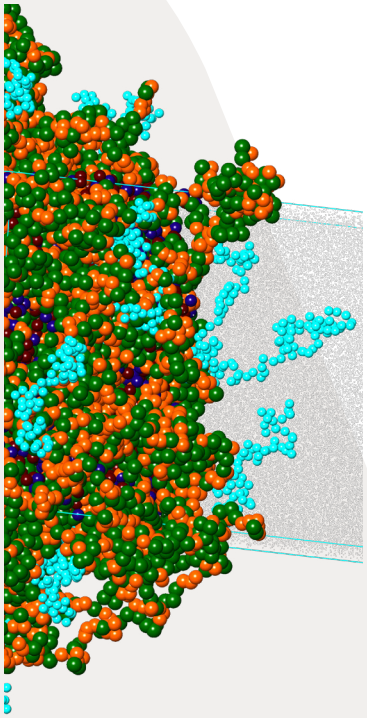
Critical phenomena for formulation and chemistry development such as phase separation and liquid structuring can occur at time and length scales that are difficult to access with all-atom molecular dynamics simulation. MS CG (Materials Science Coarse-Grained Modeling) is intended for molecular dynamics simulations of larger bulk systems over a more extended period of time than all-atom models. MS CG provides an infrastructure to draw coarse-grained molecules and map from all-atom to coarse-grained structures, as well as fit and assign coarse-grained force fields.

Capabilities

- Supports various coarse-grained (CG) models:
  - Dissipative particle dynamics (DPD)
  - Martini
  - Generalized Lennard-Jones + Coulomb potential
- Provides flexible workflows to construct systems of interest with sketcher and all-atom to coarse-grained mapping
- Offers advanced solutions for thermophysical, mechanical, and diffusion properties
- Provides different levels of particulation, from coarser models with tens of atoms per bead to finer grained models with 2-10 atoms per bead
- Integrates with other solutions and builders (e.g. Polymer Builder, Structured Liquid Builder, Stress Strain, Thermophysical Properties, Polymer Chain Analysis, Structure Factor) and other products (e.g. MS Transport)

Associated Product: Desmond





MS Penetrant Loading

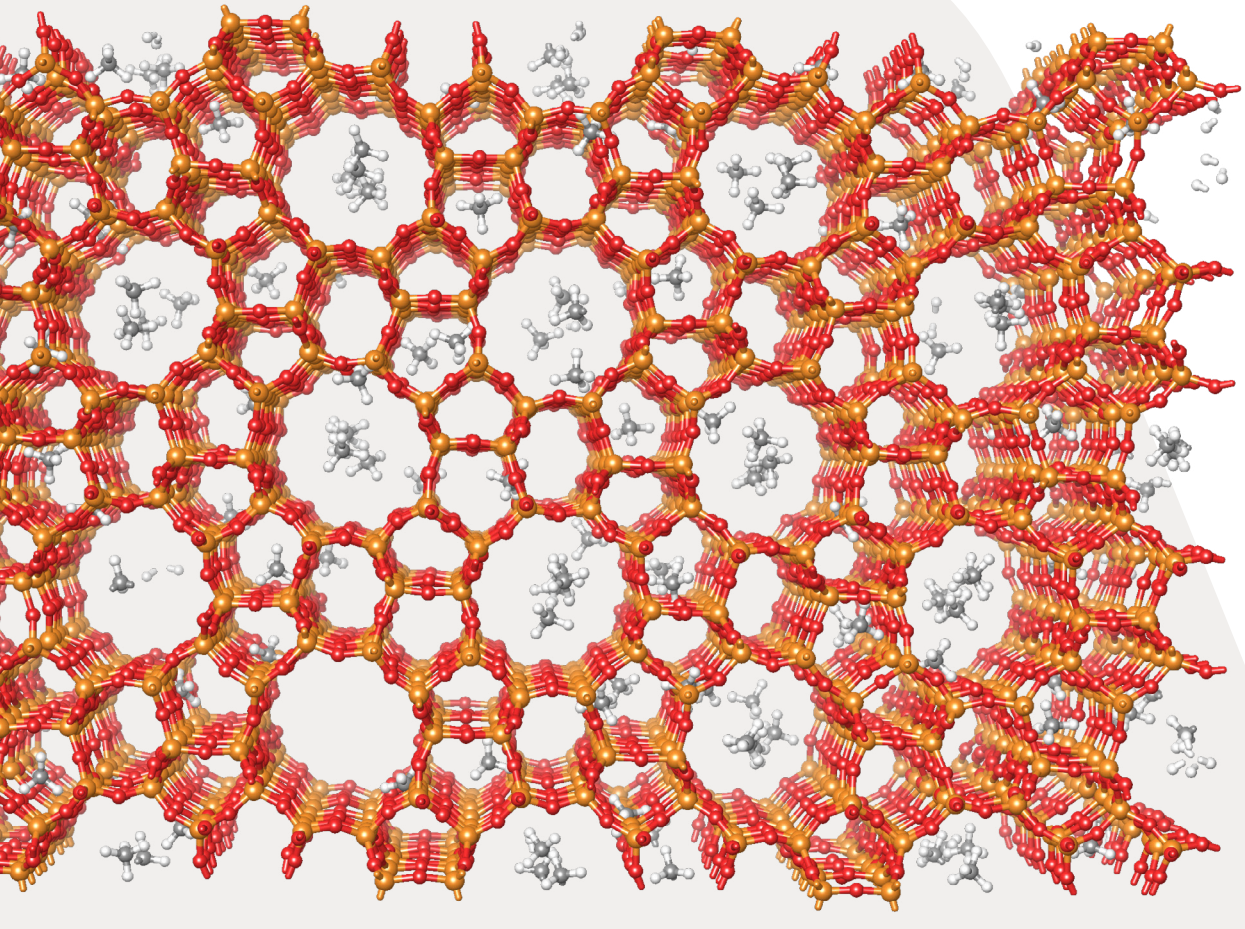
MS Penetrant Loading allows simulations of the loading of a condensed system such as a polymer, zeolite, or molecular solid by a small rigid molecule such as water or methane. The calculation provides a measure of the hygroscopicity or loading capacity of the condensed phase.

It runs Grand Canonical Monte Carlo (GCMC) simulations in Desmond, allowing for the combination of Monte Carlo and molecular dynamics for substrate relaxation. This results in more realistic loading while allowing for the quick screening of materials for equilibrium adsorption.

Capabilities

- Calculates small molecule adsorption into solid or liquid materials using Grand Canonical Monte Carlo combined with NVT or NPT MD
- Calculates uptake of water at varying temperatures and humidities
- Views results in standard experiment formats such as % uptake and % volume change
- Provides access to high speed simulation workflows with Desmond GPU
- Considers the impact of water on properties such as glass transition
- Provides insights into the swelling of materials during water uptake

Associated Product: Desmond



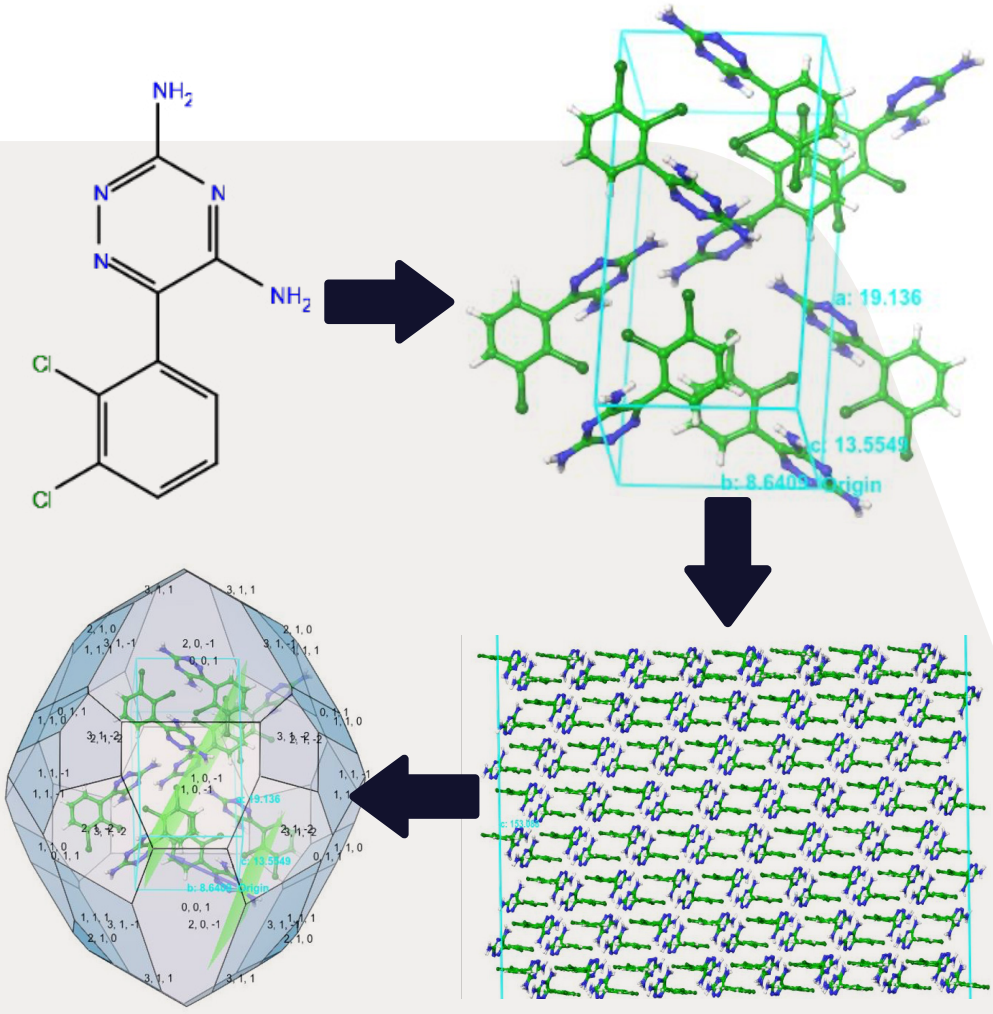
MS Morph

Crystal morphology critically affects many aspects of drug formulation and manufacturability. To some extent it can be controlled by a suitable choice of solvent and additives and crystallization conditions, such as temperature and supersaturation. Optimized crystal morphology helps to Increase the efficiency of the filtration process of the active pharmaceutical ingredient (API), improve product purity and tabletability, improve API bioavailability, optimize drying, packaging, handling and storage, and comply with toxicity requirements. MS Morph predicts crystal shape (or habits) for molecular crystals based on the surface energies and Wullf's theorem. It provides valuable insights for crystal growth mode and powder processing.

Capabilities

- Utilizes MD simulations for calculation and ranking of surface energies for a set of Miller indices
- Predicts equilibrium shape of crystallites based on relative surface energies and Wulff's theorem

Associated Product: Desmond



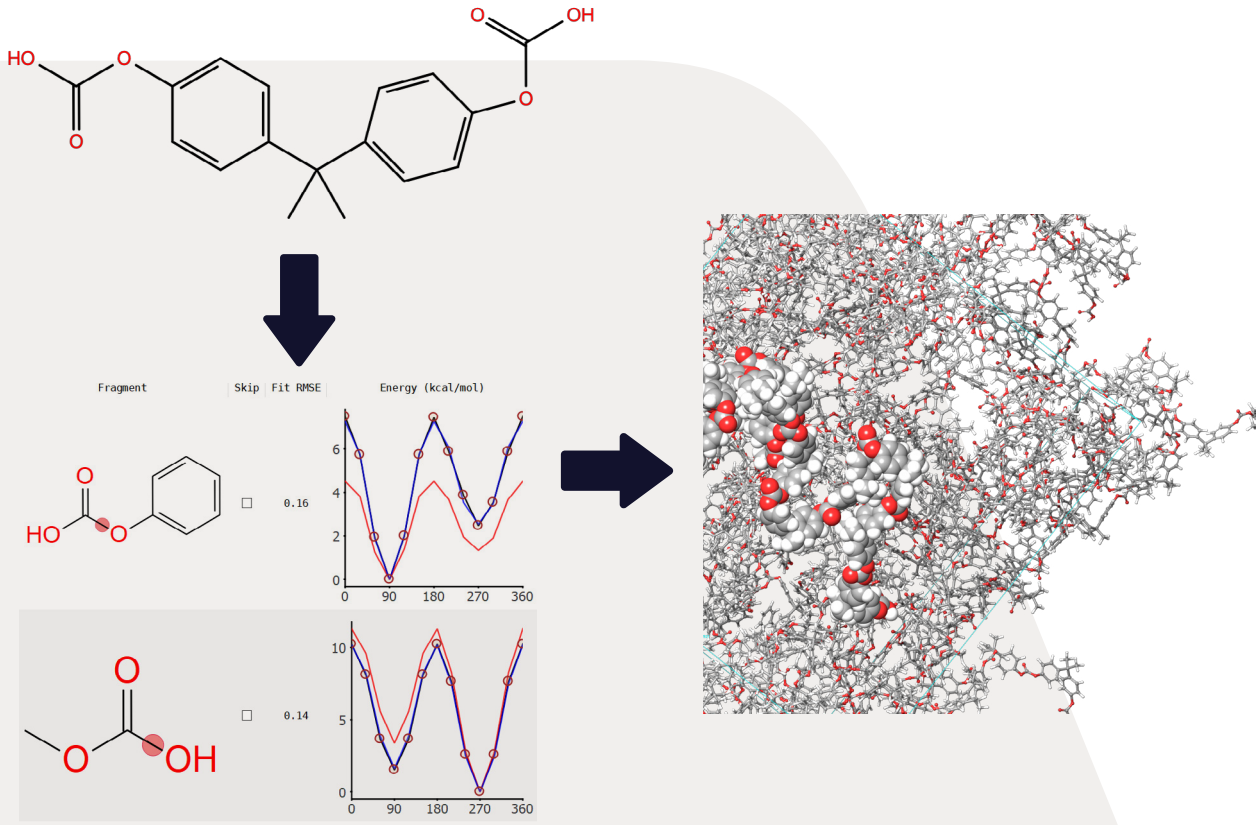
Force Field Builder

Force Field Builder is designed to provide force field parameters for torsions that are not explicitly represented in the force field. The set of molecules is analyzed to locate such torsions, and then quantum mechanical calculations are performed to obtain parameters for the torsions. New parameters are seamlessly integrated into the OPLS4 parameters directory for easy use in subsequent simulations.

Capabilities

- Builds and optimizes custom torsion parameters for previously undefined bond dihedrals
- Visualizes forcefield torsion energy profile compared to quantum mechanical profile

Associated Products: Jaguar, MacroModel



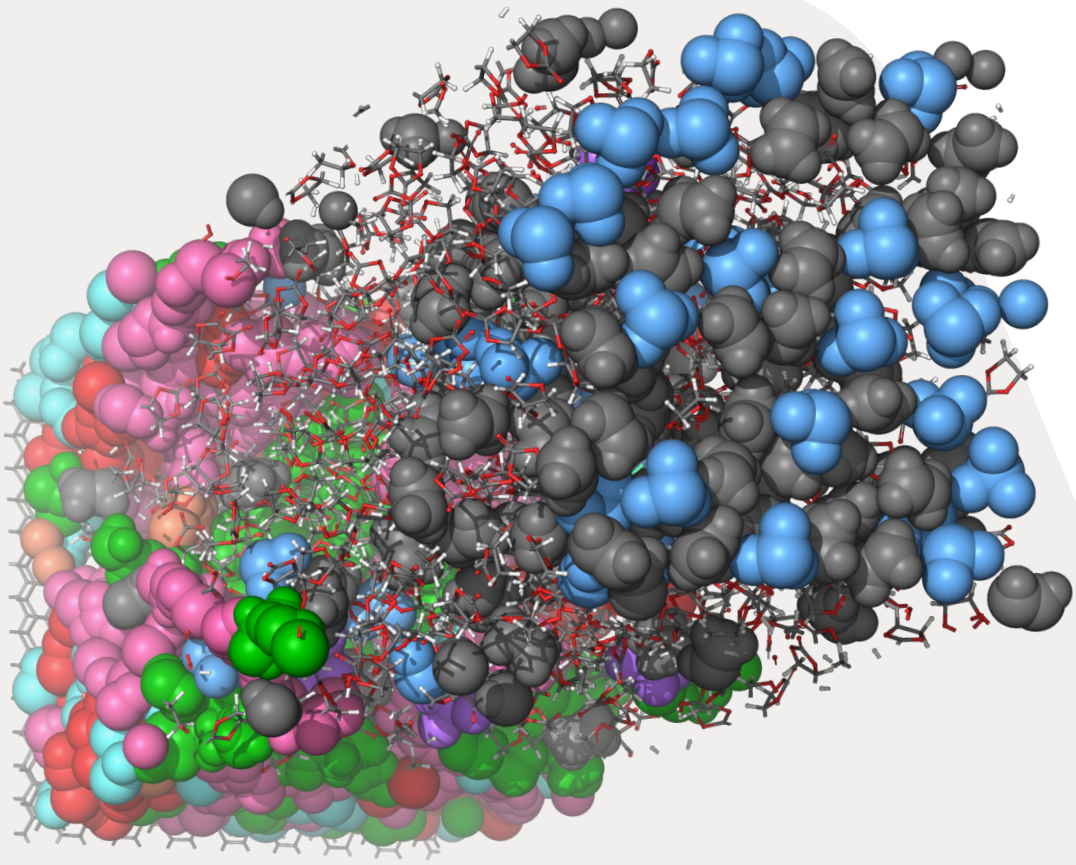
MS Reactive Interface Simulator

MS Reactive Interface Simulator enables rapid modeling of solid electrolyte interphase (SEI) nucleation and growth in batteries using a template-based reaction approach, and offers atomistic insights into the composition and morphology of this complex battery component. Coupled with Desmond, Schrödinger's high-speed GPU-based molecular dynamics (MD) engine, and the OPLS force field, MS Reactive Interface Simulator facilitates efficient analysis of electrolyte chemistries by generation of realistic SEI morphologies.

Capabilities

- Accelerates physically realistic SEI formation with GPU-accelerated MD
- Executes reactions using predetermined templates
- Enables exploration of multiple chemistries under varying conditions with SMARTS based reaction templates
- Employs advanced analysis tools to characterize morphology and understand the properties of the SEI layer

Associated Product: Desmond



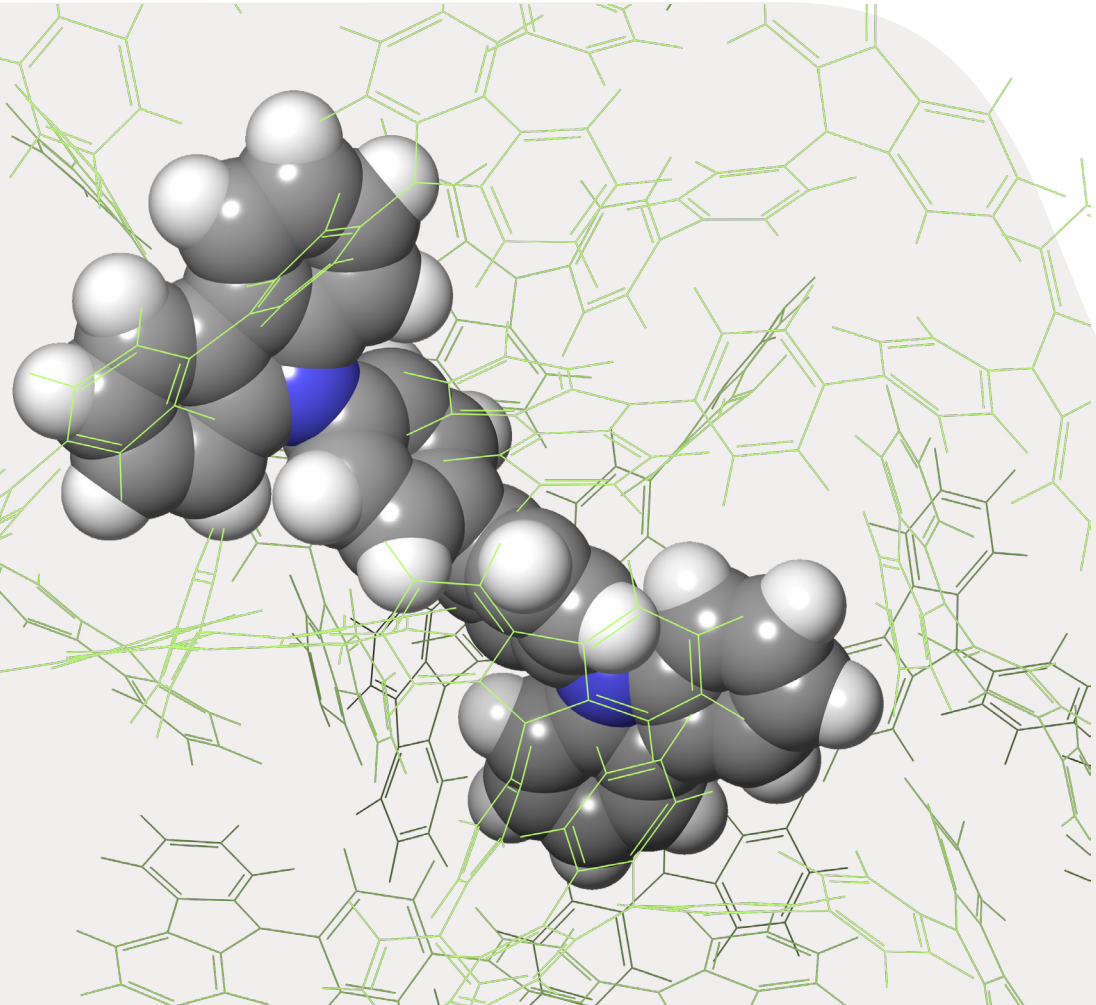
Multiscale

QSite

QSite is a multi-scale simulation tool that utilizes the QM/MM method, which combines the principles of quantum mechanics and molecular mechanics. It is designed to accurately predict the molecular configurations, energetics, and the electronic structures of a reactive system through quantum chemical treatment of atoms, providing crucial insights into reactive chemistry essential for understanding chemical transformation in the presence of intermolecular interactions. QSite is equally applicable for describing non-reacting chemical systems.

Capabilities

- Performs QM/MM calculations for quantum chemical treatment of large molecules (such as crystals and proteins)
- Supports a wide range of DFT functionals
- Offers coordinate scans with atom constraints



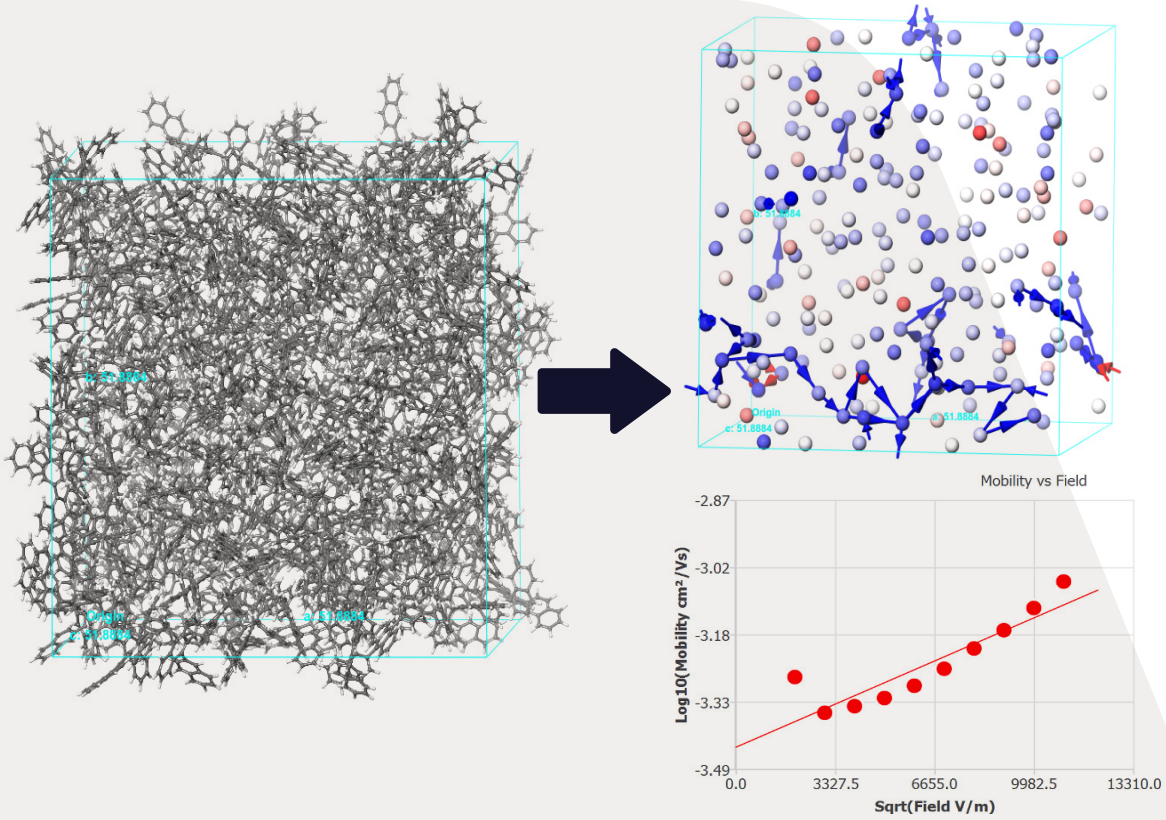
MS Mobility

MS Mobility utilizes Marcus rate theory and kinetic Monte Carlo (KMC) approach to analyze factors affecting charge mobility in amorphous and crystalline solids. The module automatically analyzes the provided solid morphology and calculates all necessary quantum mechanical parameters. The calculated parameters are passed into the KMC calculations or stored for further calculations and analysis.

Capabilities

- Predicts charge carrier mobility for molecular semiconductors based on Marcus rate theory and KMC
- Assesses impact of electric field, temperature and charge carrier concentration
- Calculates electron and hole hopping rates based on Marcus rate theory
- Analyzes mobility as function of field direction, temperature, and charge carrier concentration
- Allows visualization of percolation path and charge traps and their relation to a local morphology

Associated Products: Jaguar, QSite



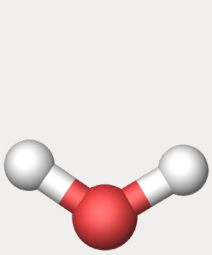
MS Dielectric

MS Dielectric employs both Jaguar quantum mechanics (QM) and Desmond molecular dynamics (MD) calculations to obtain key optical and dielectric properties. With simple settings and input of only a single molecule or polymer monomer, all the subsequent system building, simulations, and analyses are performed automatically.

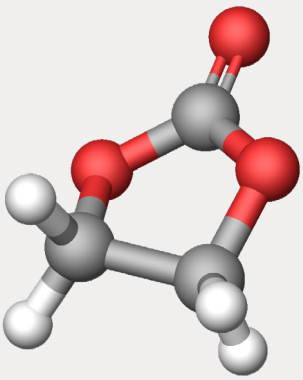
Capabilities

- Computes dielectric properties of molecular materials with combined quantum mechanical and molecular dynamics solutions
- Calculates the refractive index, Abbe number, and static dielectric
- Simulates and plots complex dielectric constant with dielectric loss versus frequency

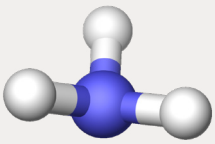
Associated Products: Desmond, Jaguar



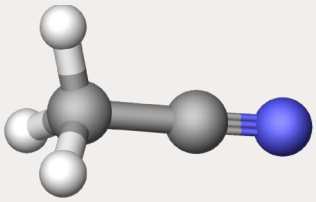
water: 1.32



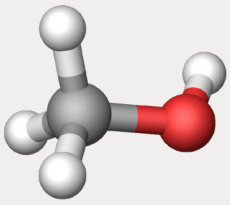
EC: 1.42



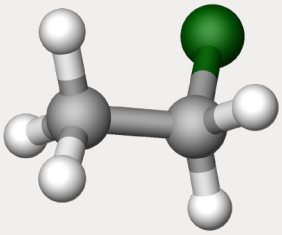
ammonia: 1.29



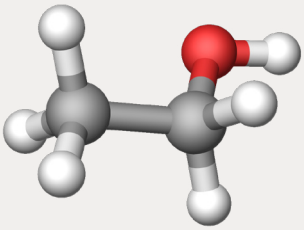
acrylonitrile: 1.31



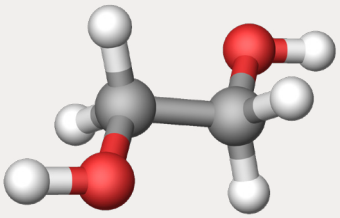
methanol: 1.31



chloroethane: 1.35



ethanol: 1.35



ethylene glycol: 1.41

MS Microkinetics

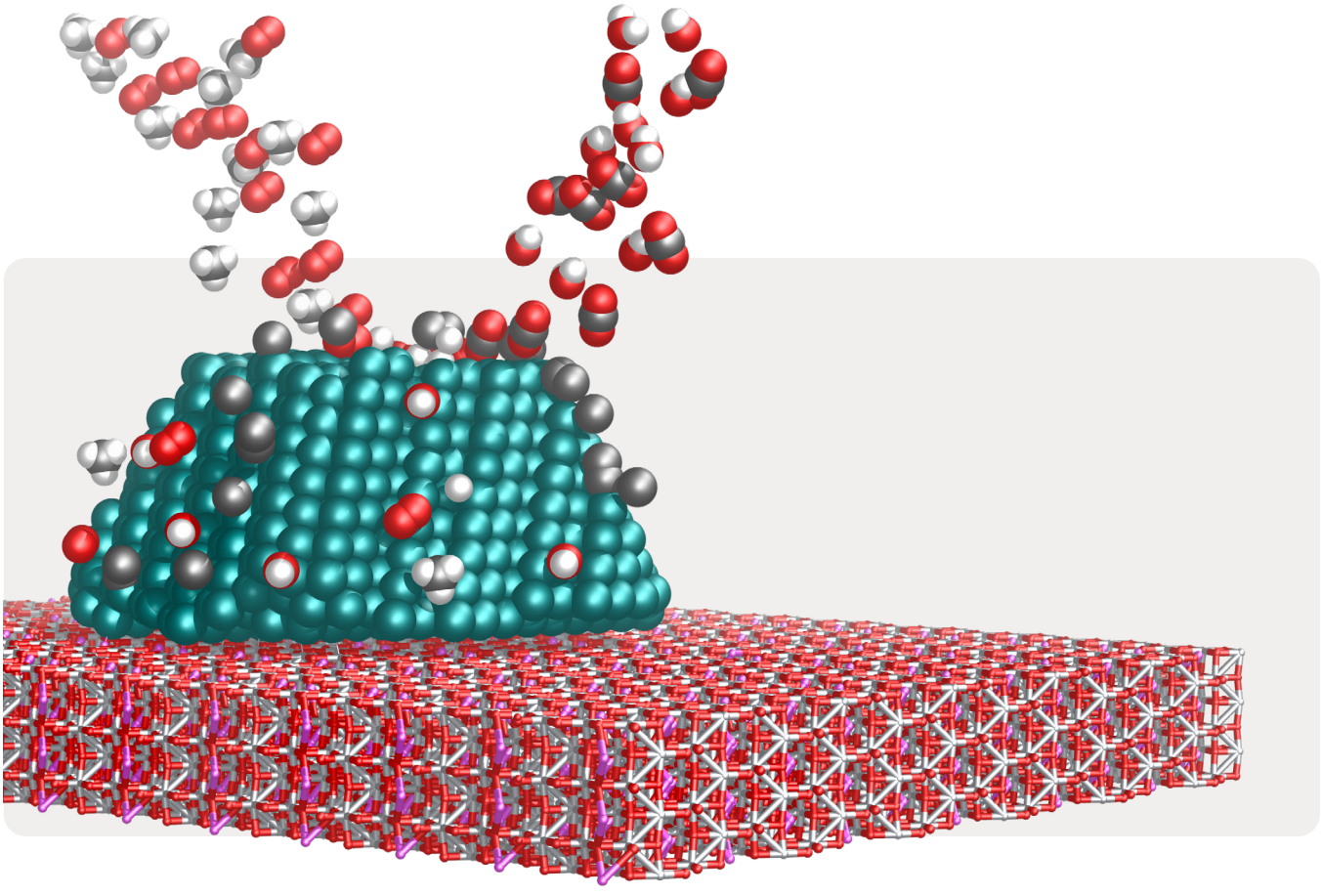
MS Microkinetics is an effective tool for calculating the overall kinetics of a network of surface reactions, which can be used to optimize reaction conditions and to identify reactivity bottlenecks.

Capabilities

Given the reaction mechanism (or multiple mechanisms) and activation free energies, MS Microkinetics calculates:

- Reaction rates for the elementary reaction steps
- Time-dependent and steady state coverages of the reactants, products, and intermediates
- Reaction orders
- Degree of rate control
- Turnover frequency in the case of catalytic cycles
- Growth rate or etch rate in the case of deposition or etch processes

Associated Products:
Jaguar, Quantum ESPRESSO Interface



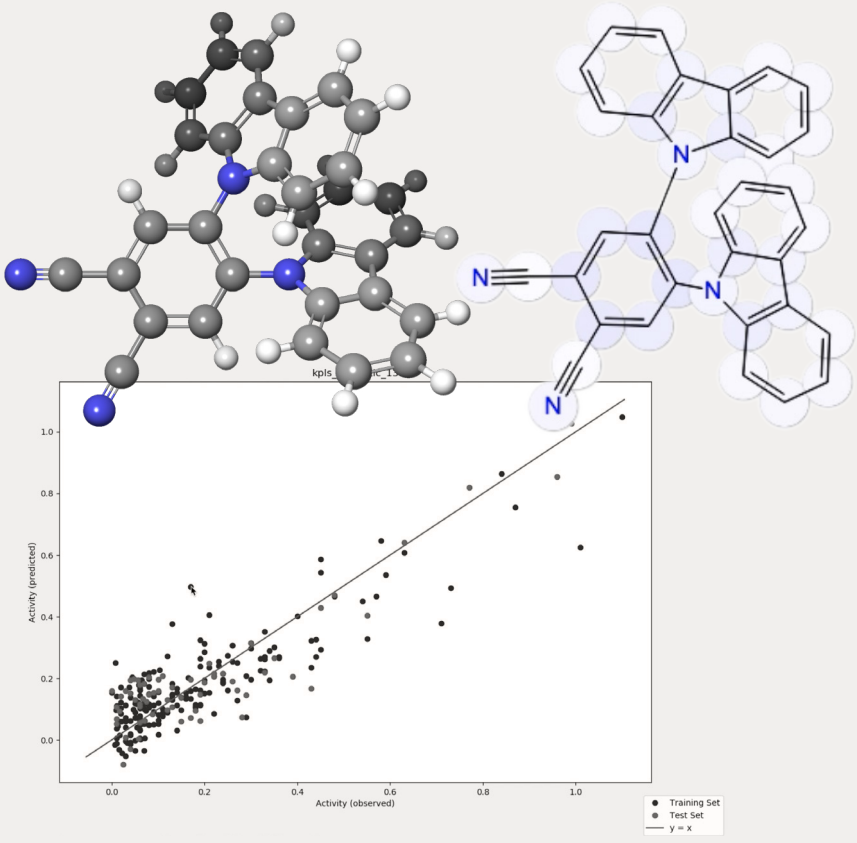
Machine Learning

Deep AutoQSAR

DeepAutoQSAR is a machine learning (ML) solution that allows users to predict molecular properties based on chemical structure. The automated supervised learning pipeline enables both novice and experienced users to train and inference best-in-class quantitative structure activity/property relationship (QSAR/QSPR) models.

Capabilities

- Takes 1D, 2D, or 3D structural data as input and a desired property to be modeled and automatically computes descriptors and fingerprints
- Creates QSAR/QSPR models with multiple machine learning statistical methods, evaluates each QSAR/QSPR model for predictive accuracy, and rank orders all the QSAR models by their predictive power
- Supports deep neural network based predictions and fully exploit large datasets with integration of DeepChem

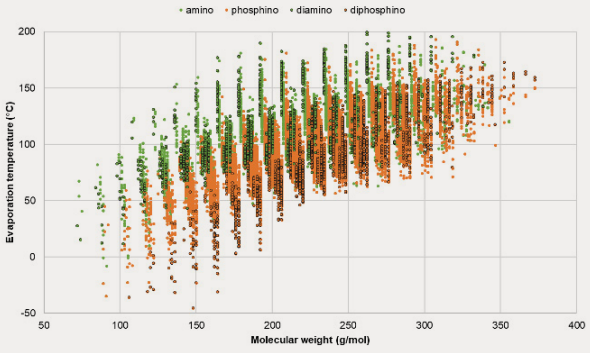


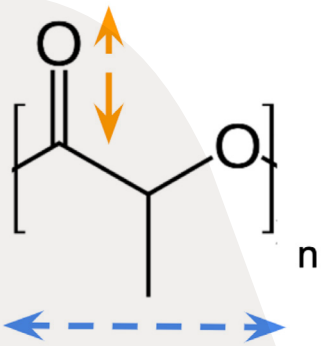
MS Informatics

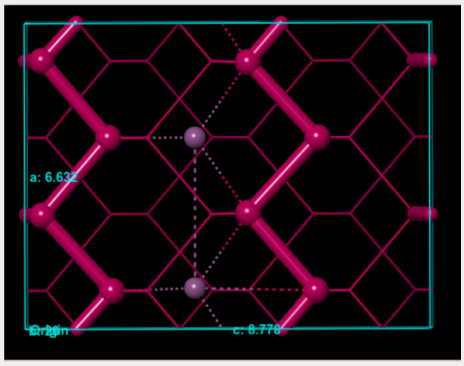
MS Informatics provides molecular featurization and machine learning (ML) tools for organic, organometallic, polymer, chemical mixture (i.e., formulation), and inorganic solid materials to help design new materials through data driven approaches. By combining physics-based featurization, customized pretrained ML models, and automated workflows to train and evaluate ML models, users can take advantage of the computationally efficient data-driven approaches to screen and down select promising materials.

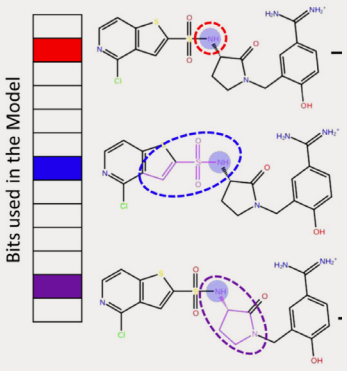
Capabilities

- Analyzes structures and diversity of a large chemical space with cheminformatics tools
- Generates advanced (2D/3D/repeat-unit-based) descriptors for organic, inorganic, and polymeric materials
- Offers featurization by QM and semiempirical QM molecular descriptors
- Provides model building tools for quantitative structure-property relationship (QSPR)
- Supports machine learning models built for repeat-unit-based polymer representations
- Builds formulation-property models for chemical mixtures with varying ingredient structures and compositions
- Includes pre-built machine learning models for various key properties, e.g. boiling point and vapor pressure, Tg of polymers, frequency-dependent polymer dielectric constant and dielectric loss, density of small molecules, and optoelectronic properties









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