Materials Science Product Guide

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

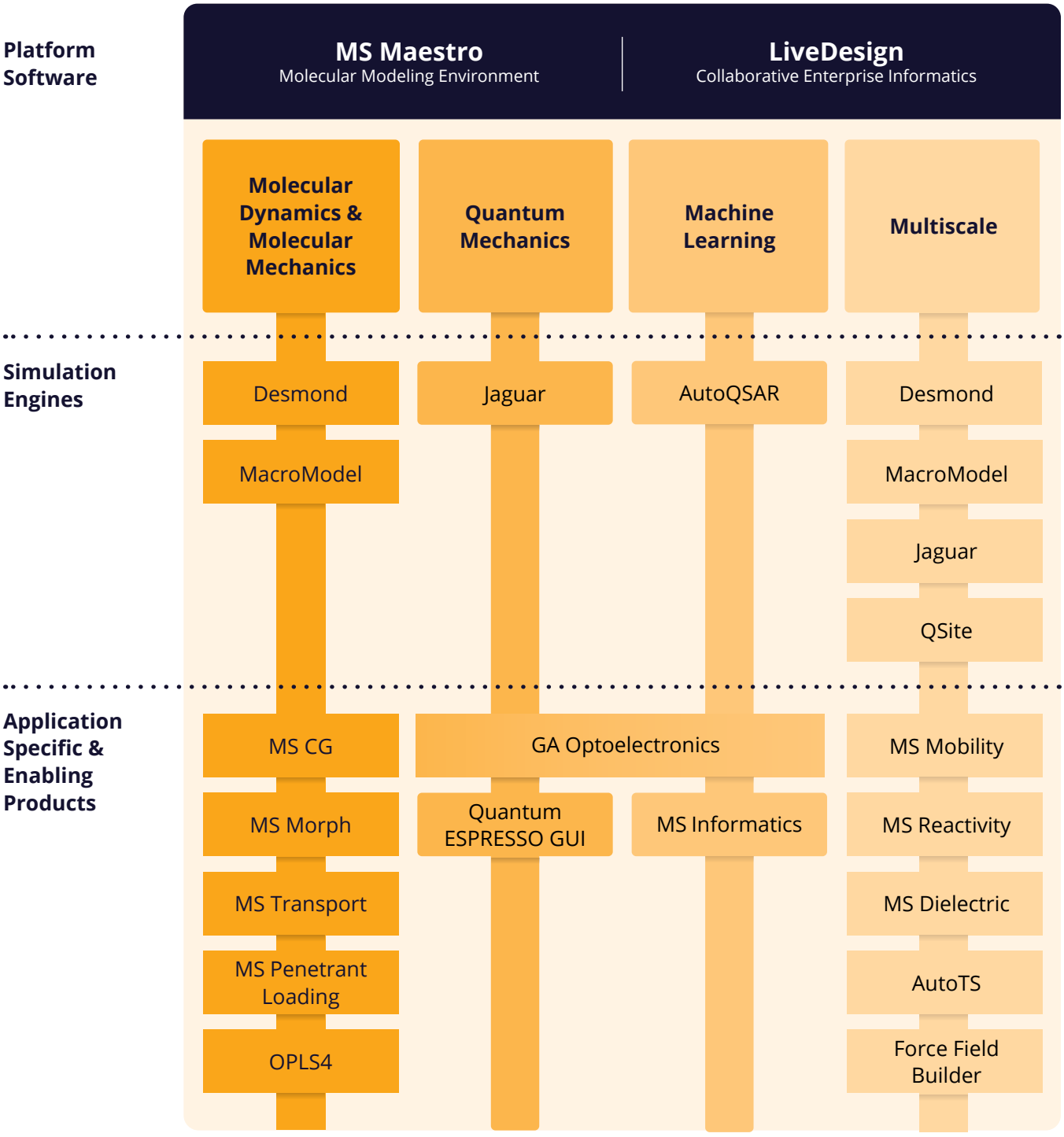
Schrödinger | Materials

Applications

Schrödinger's Materials Science solutions offer unprecedented insights into the mechanisms and properties of materials and chemical systems in a wide range of technological applications:

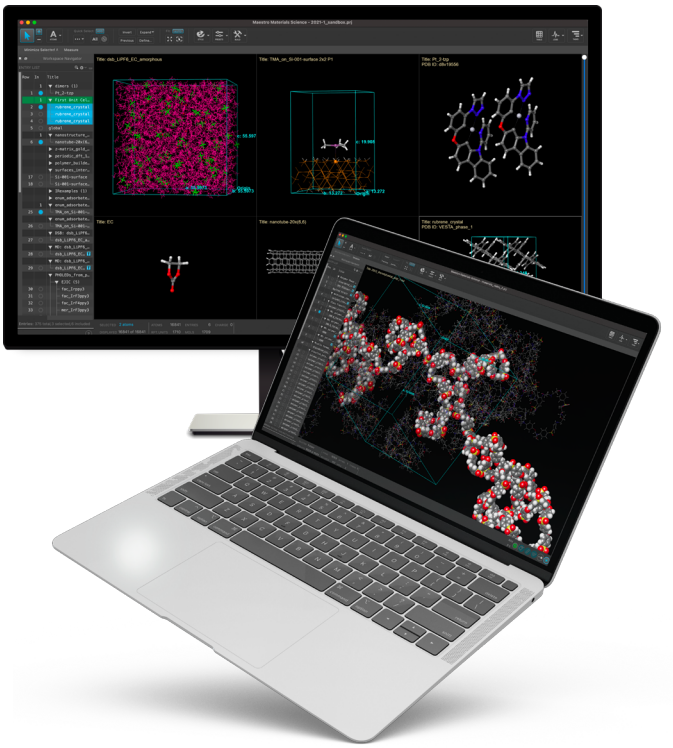
- Organic Electronics
- Polymeric Materials
- Consumer Packaged Goods
- Catalysis & Reactive Systems
- Semiconductors
- Energy Capture & Storage
- Complex Formulations
- Metals, Alloys & Ceramics

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 unified and integrated modeling environment
- Builds realistic structural models of crystals, organometallic complexes, polymers, slabs and interfaces, and more with advanced structure builder
- Accesses advanced machine learning and cheminformatics tools and solutions for predictive model building and validation
- Offers combinatorial chemistry solutions with structural enumeration and automated library generation
- Provides comprehensive data analysis tools pipelined to materials modeling and simulations through chemically-aware spreadsheet environment
- Manages large-scale computational modeling & simulation tasks on local / remote compute servers across Linux, Windows, Mac and cloud
- Includes additional key features: optoelectronics workflow solutions, advanced model building and simulation modules for polymers and plotting & multivariate optimization tools

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, and 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 non-experts
- 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 collective learning

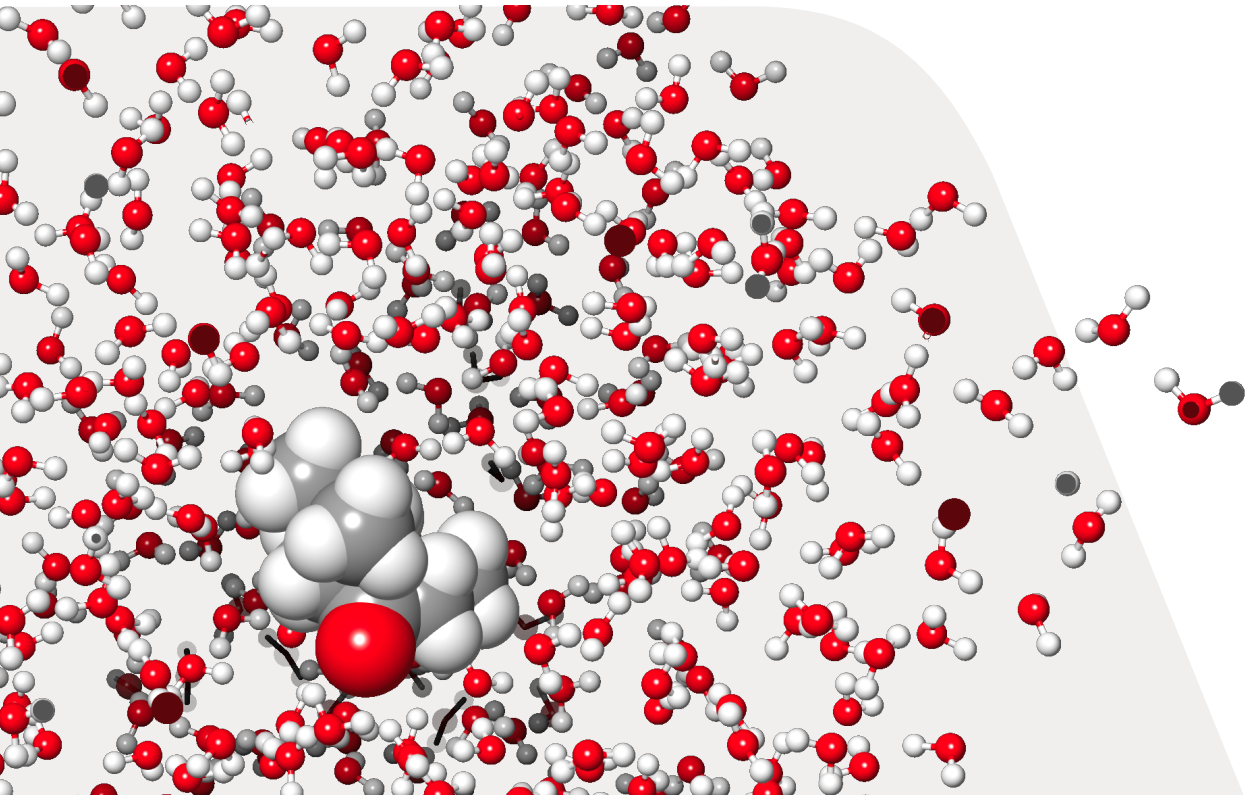
Molecular Dynamics & Molecular Mechanics: Engine

Desmond

Desmond is a GPU-powered high-performance molecular dynamics (MD) engine providing high scalability, simulation throughput, and scientific accuracy to predict bulk properties of materials, such as thermophysical properties, elastic constants, stress/strain relationships, diffusion coefficients, viscosity, persistence length, etc. It enables the capability required to establish a "Materials by Design" framework in a broad range of industries.

Capabilities

- Improves computing speed by 100x on general-purpose GPU (GPGPU) versus single CPU
- Simulates single component, 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, Meta-dynamics, and Simulated Annealing
- Supports coarse-grained force fields (with MS CG), incorporating all Desmond capabilities to coarse-grained modeling

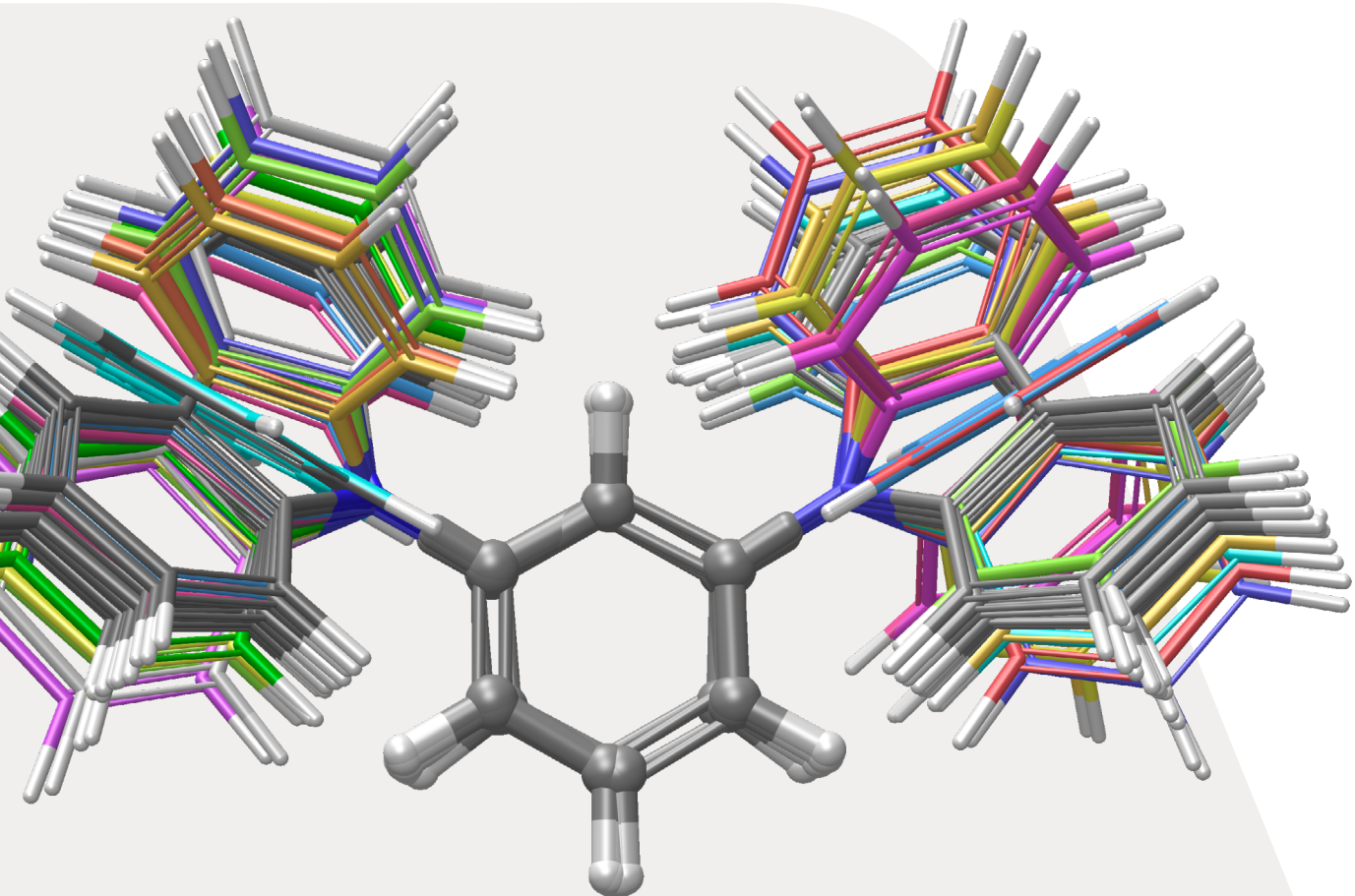


MacroModel

MacroModel is a general purpose, force-field-based molecular modeling program with applicability to a wide range of chemical systems. It provides researchers with multiple advanced methods to aid the understanding of chemical structure, energetics, and dynamics. MacroModel is routinely applied to examine molecular conformations, molecular motion, and intermolecular interactions for a wide range of different materials including organic and inorganic molecules and oligomers, organometallic complexes as well as 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, OPLS_2005 and OPLS4



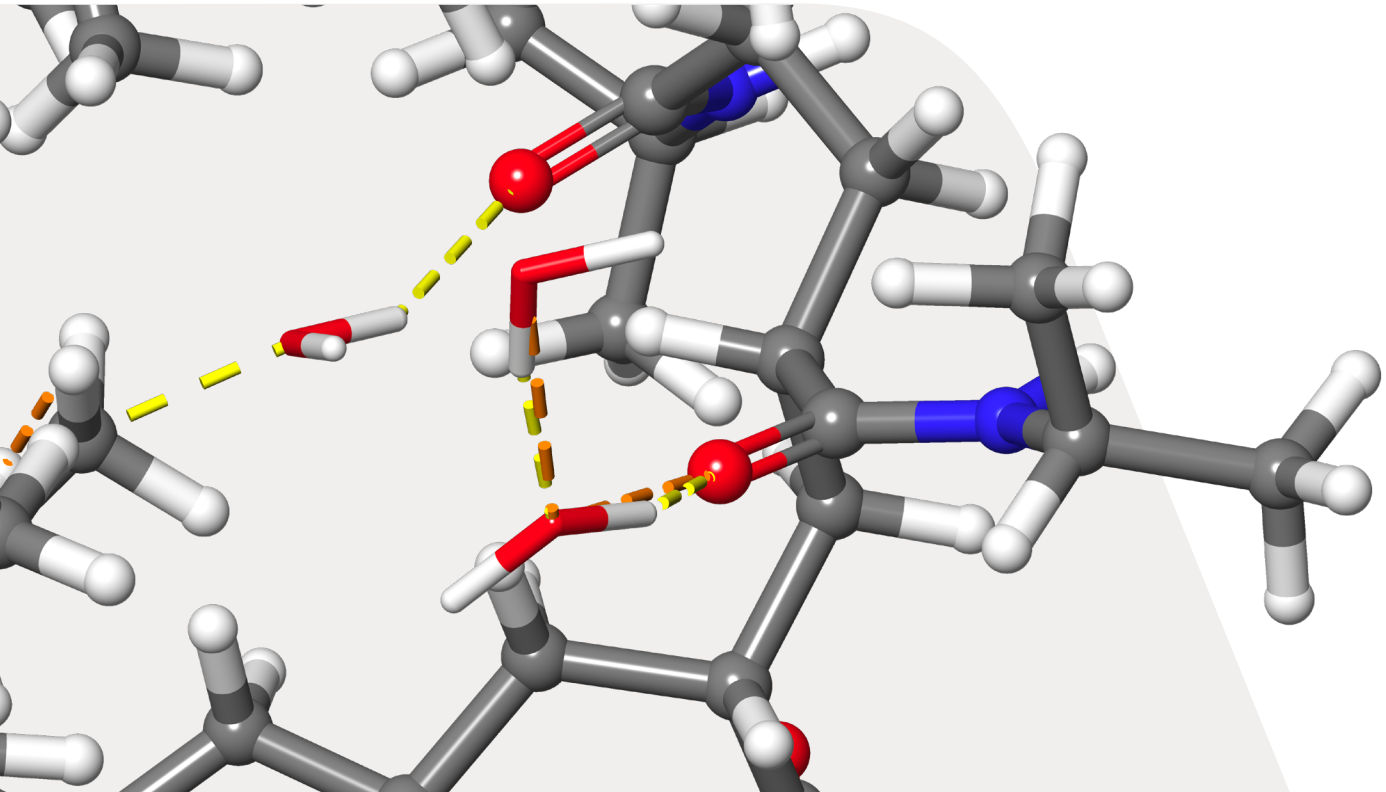
Molecular Dynamics & Molecular Mechanics: Force Field

OPLS4

Accurate force field parameters are at the heart of obtaining useful molecular structures and relative energies for practical use in material design and developments. OPLS4 is the latest version of Schrödinger's modern force field. It offers proven performance for small molecules, organics, polymers, OLEDs, silicates, and more, providing coverage for numerous industries. OPLS4 provides leading accuracy through detailed parameterization.

Capabilities

- Offers commercial-grade force field for classical MD and organic materials design
- Contains small molecule torsion parameter coverage of 95% for relevant chemical space
- Offers over 100k 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



Molecular Dynamics & Molecular Mechanics: Products

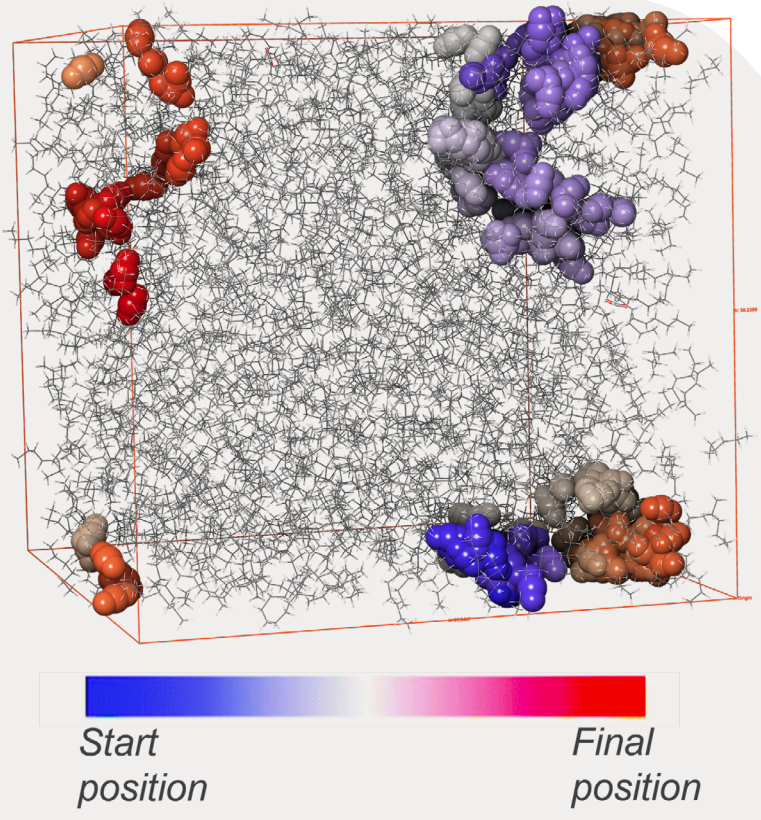
MS Transport

MS Transport provides access to 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 Desmond speed to calculate diffusion and viscosity in industrially relevant clock times
- Calculates diffusion of gases through matrices, ions through battery polymers, and additives in plastics with focused workflow and analysis viewer
- Predicts viscosity with latest in equilibrium molecular dynamics approaches
- Calculates transport properties at desired temperatures and explore the temperature dependence of diffusion and viscosity
- Visualizes diffusion and viscosity plots

Associated Product: Desmond



MS CG

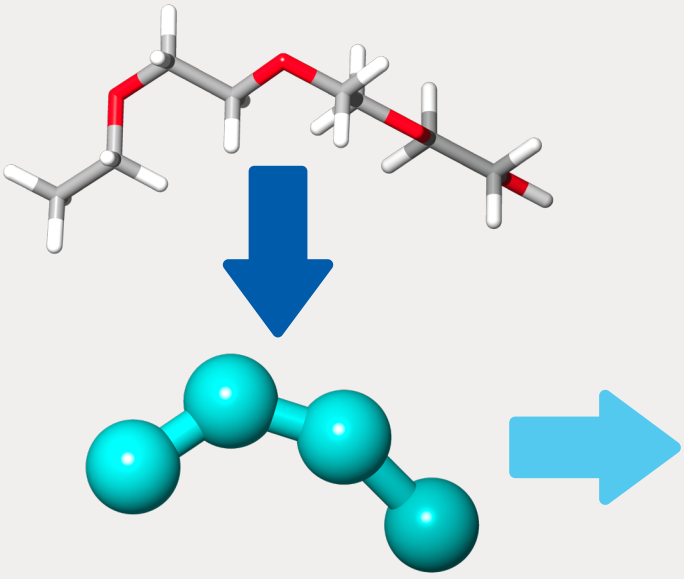
Critical phenomena for formulation and chemistry development such as phase separation and liquids structuring can occur at time and length scales that are difficult to access with all atom simulation. MS CG (Materials Science Coarse Grained Modeling) is intended for molecular dynamics simulations of larger bulk systems over a more extended period of time than all-atom (AA) models.

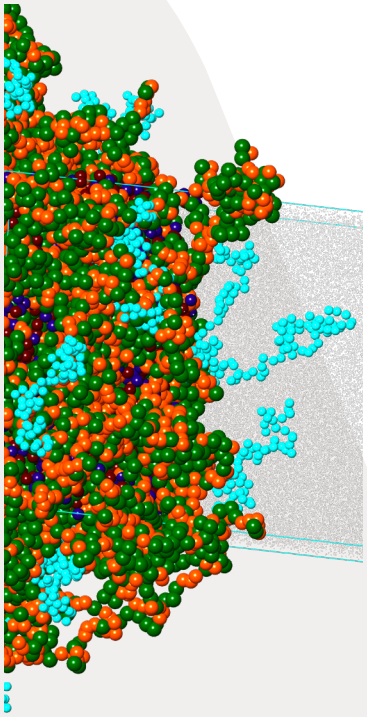
MS CG provides an infrastructure to draw Coarse-Grained molecules, map from all-atom to Coarse-Grained structures, and assign Coarse-Grained force fields. Coarse-Grained dynamics are also faster with the reduction in atomistic detail making it possible to study behavior extending beyond the typical atomistic simulation time.

Capabilities

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

Associated Product: Desmond





MS Penetrant Loading

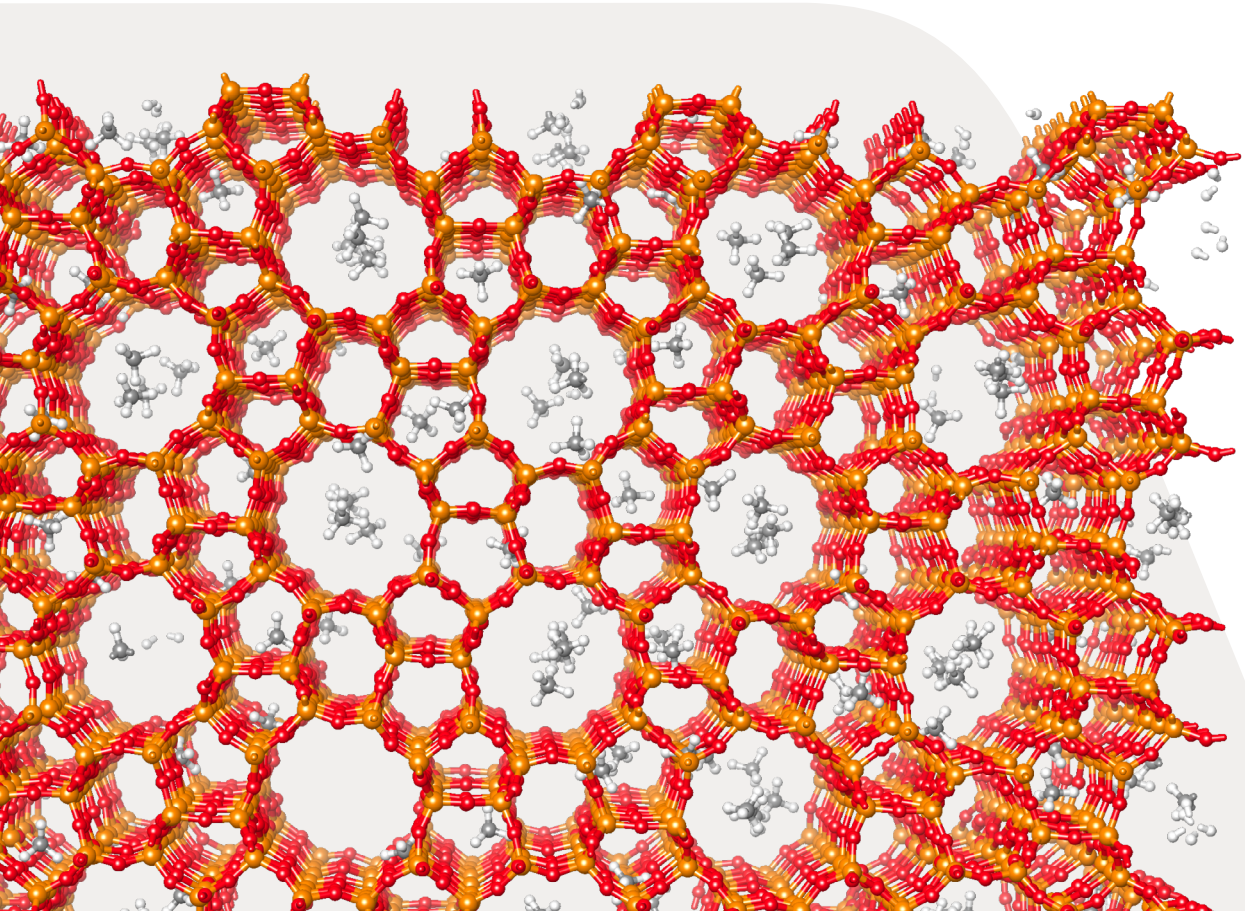
MS Penetrant Loading allows simulations of the loading of a condensed system such as a polymer, zeolite, or molecular solid by a small rigid molecule such as water or methane. The calculation provides a measure of the hygroscopicity or loading capacity of the condensed phase.

MS Penetrant Loading runs GCMC in Desmond allowing for the combination of Monte Carlo and MD for substrate relaxation resulting in more realistic loading, 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 Molecular Dynamics
- 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



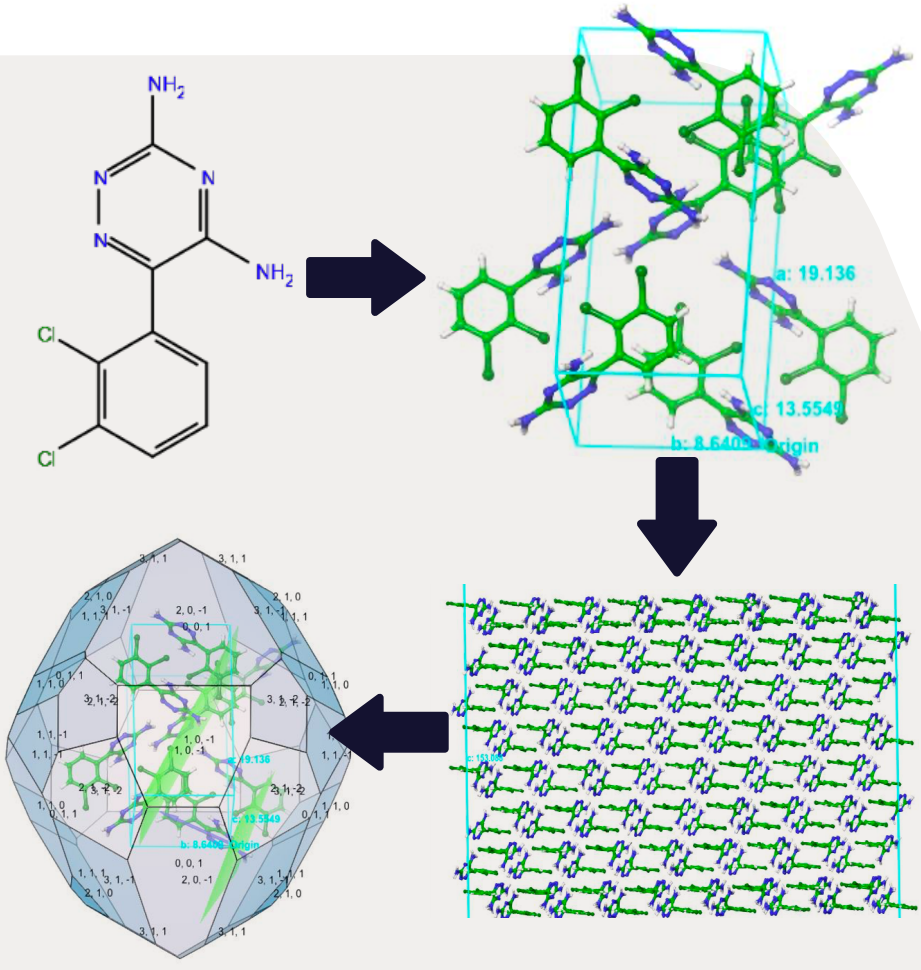
MS Morph

MS Morph predicts crystal shape for molecular crystals based on the surface energies and Wulff's theorem. It provides valuable insights for crystal growth and powder processing.

Capabilities

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

Associated Product: Desmond



Quantum Mechanics: Engine

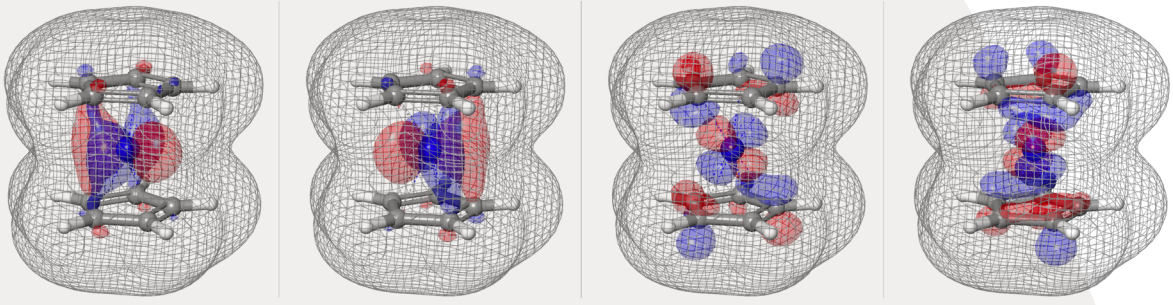
Jaguar

Jaguar specializes in fast electronic structure predictions for molecular systems of medium and large size via the use of density functional theory (DFT) based on the pseudospectral (PS) method which scales reasonably 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 – made possible by Jaguar's industry-leading efficiency and robustness.

Capabilities

- Offers a wide range of types of molecular QM calculations: geometry optimization, transition state search, thermochemical properties, implicit solvation, spectra prediction, etc.
- Provides a wide variety of DFT functionals with analytic second derivatives and dispersion corrections
- Offers sophisticated geometry constraints, rigid and relaxed scans
- Performs relativistic DFT calculations
- Provides several times speedup at a negligible loss of accuracy with optional pseudospectral approximation
- Offers automated workflows for advanced analysis: 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

Quantum Mechanics: Products

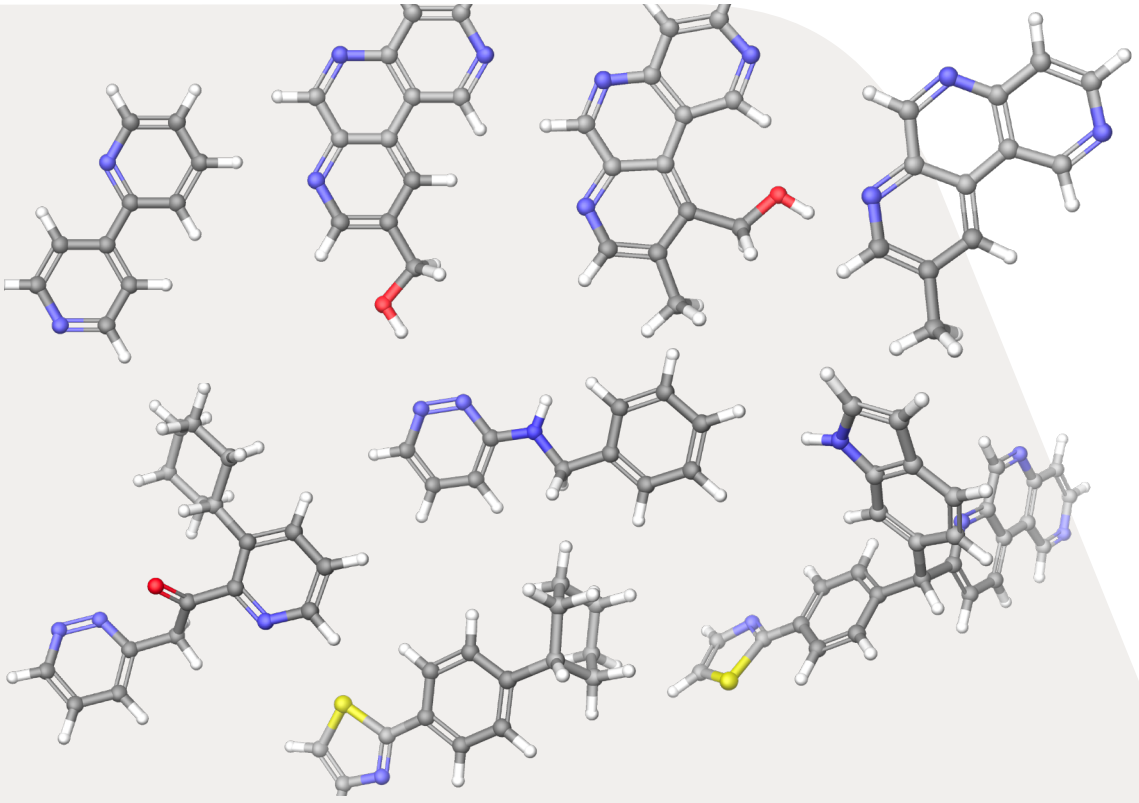
GA Optoelectronics

GA Optoelectronics enables optimization of materials properties for optoelectronic applications via a genetic algorithm. It allows the users to implement efficient screening modes using the MS Jaguar quantum mechanics engine, minimizing computational expense while delivering valuable, accurate data. 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 the target property space with genetic optimization
- Supports optimization by QM (DFT) calculated properties
- Supports optimization by model-predicted properties via machine learning
- Supports basic molecular design constraints (number of elements, molecular weight, etc.)

Associated Product: Jaguar



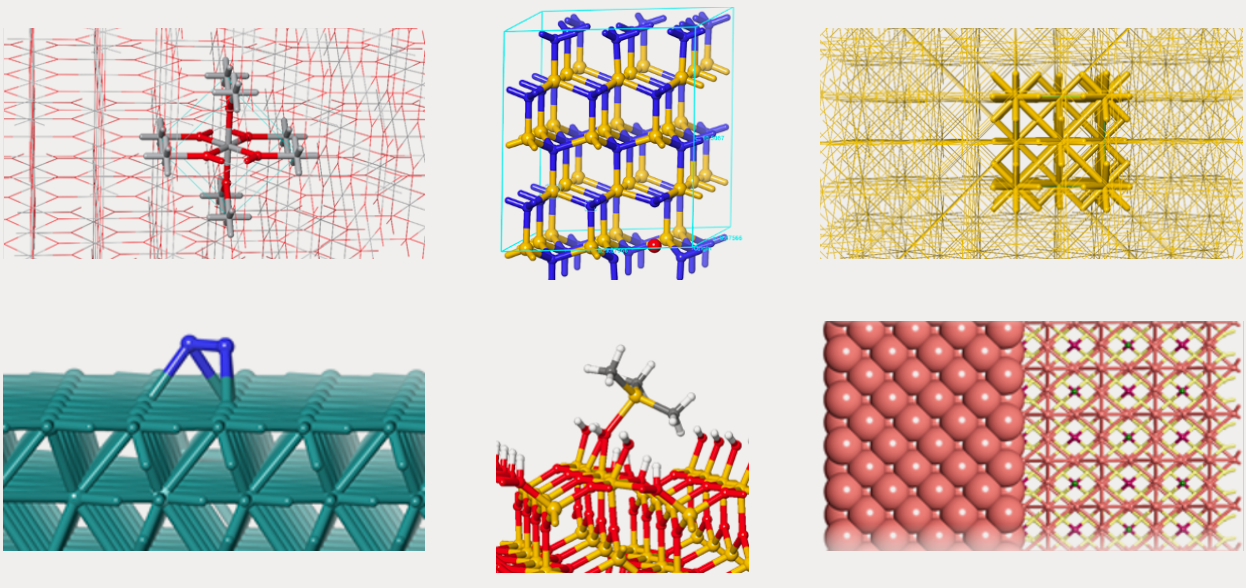
Quantum ESPRESSO GUI

Quantum ESPRESSO, developed by Quantum ESPRESSO Foundation, 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.

Quantum ESPRESSO GUI 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 Bands (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, etc.



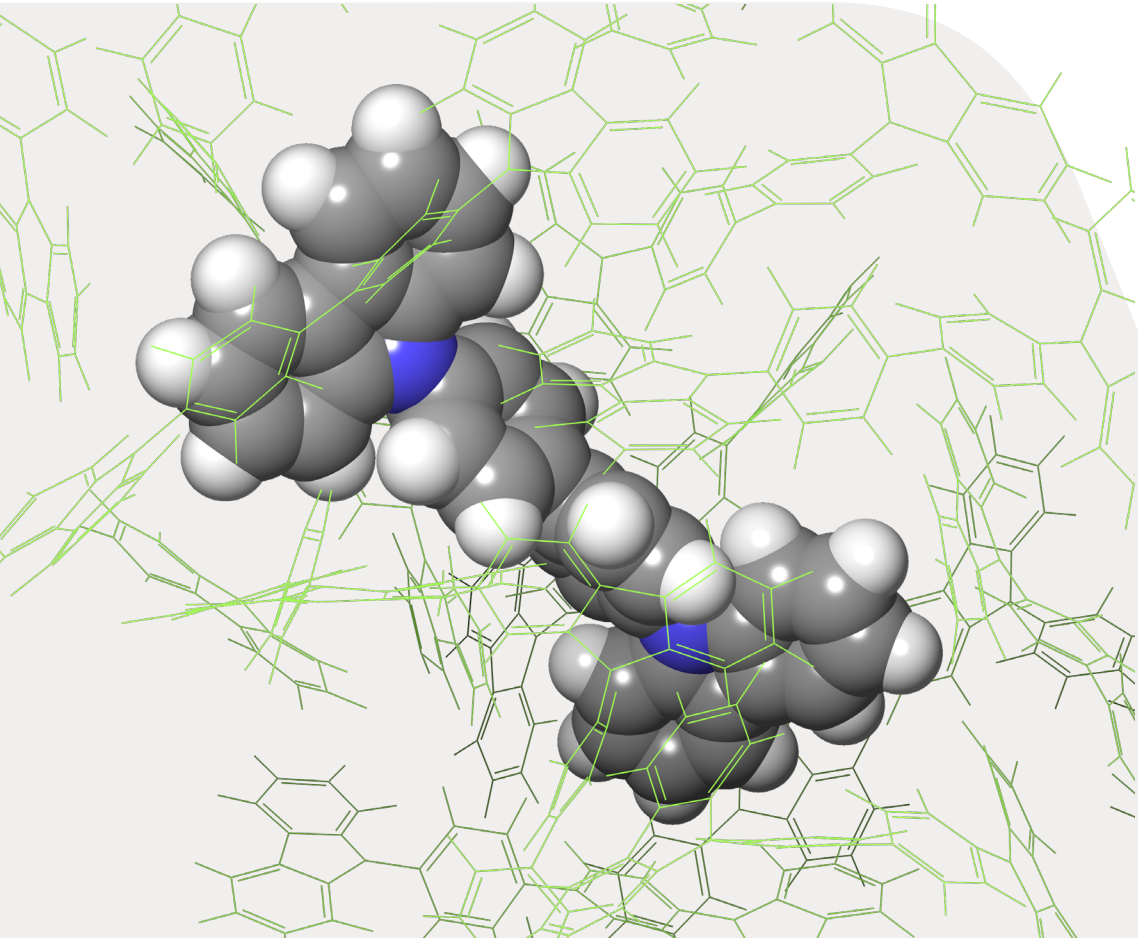
Multiscale: Engine

QSite

QSite combines the accuracy of Quantum Mechanics (QM) and the speed of Molecular Mechanics (MM) into a mixed mode QM/MM calculation. Transition metal atoms, and parts of the molecule undergoing chemical transformation require superior accuracy and are typically unsuitable for treatment with MM. QSite processes such molecular fragments with QM whereas the rest of the molecular system is described by MM.

Capabilities

- Offers a wide range of types of molecular QM 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



Multiscale: Products

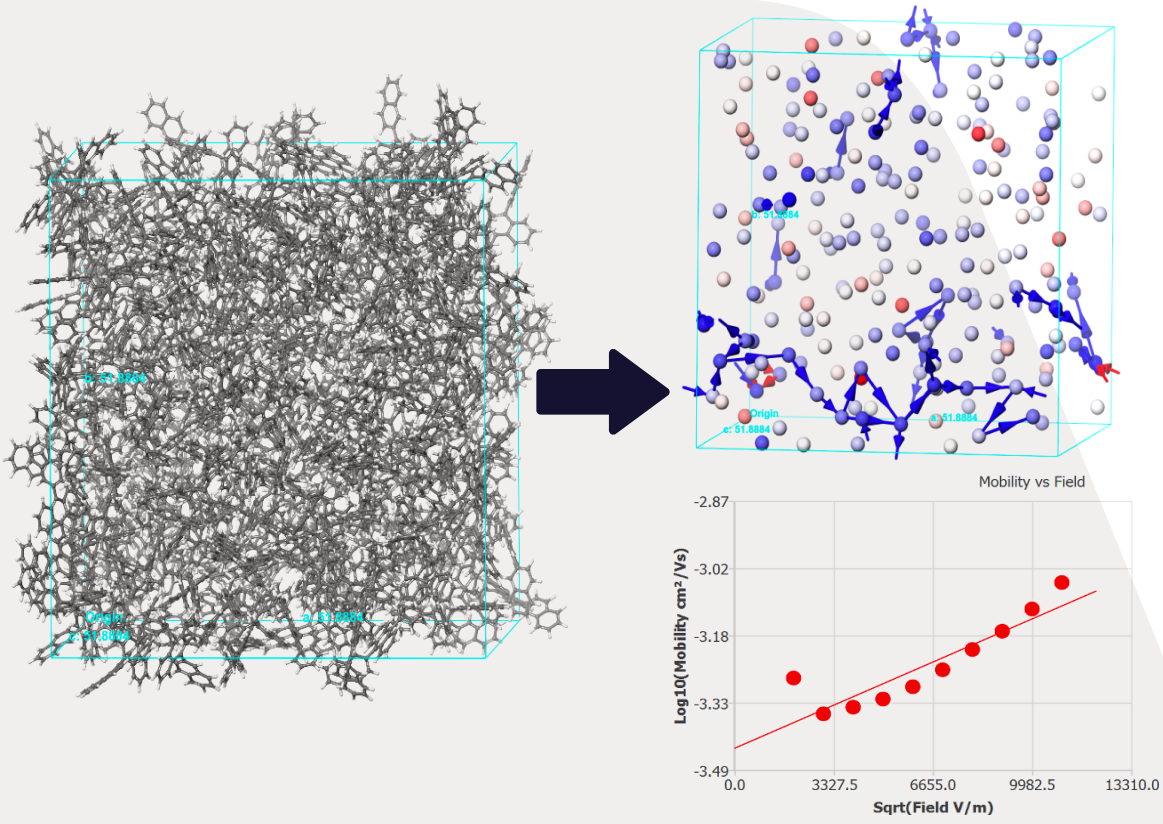
MS Mobility

MS Mobility utilizes Marcus rate theory and kinetic Monte Carlo approach to analyze factors affecting charge mobility in amorphous and crystalline solids.

Capabilities

- Predicts charge carrier mobility for molecular semiconductors based on Marcus rate theory and Kinetic Monte Carlo (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



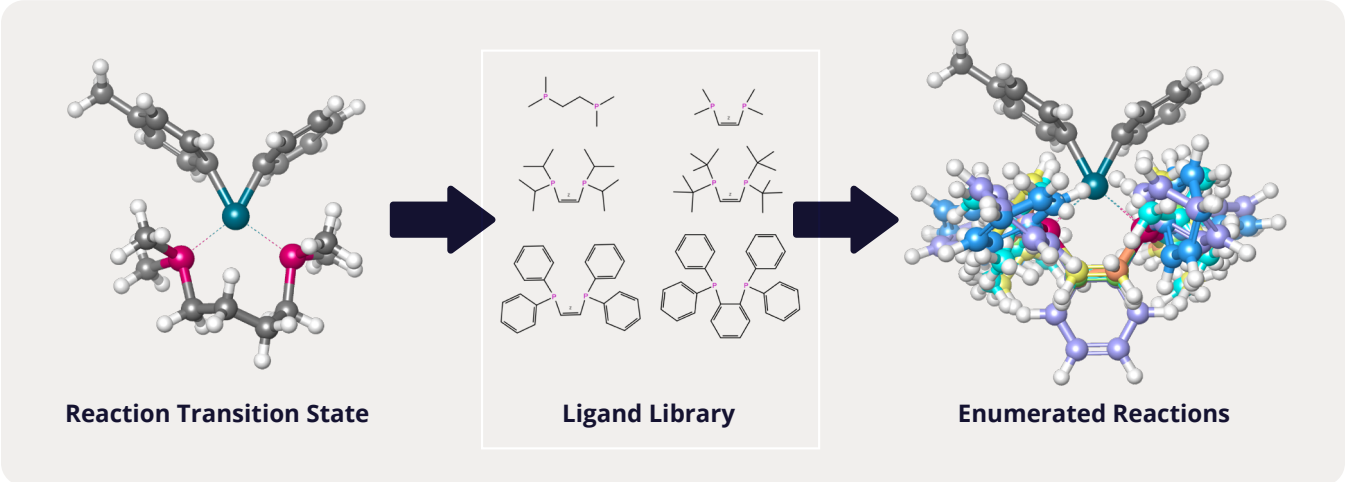
MS Reactivity

MS Reactivity offers a set of tools for reactivity and catalysis. Auto Reaction Workflow (AutoRW) facilitates the high-throughput screening of catalyst and/or substrate derivatives using a combination of enumeration tools, the Reaction Workflow (RW), and machine learning (ML) descriptor generation. The RW runs both Jaguar Density Functional Theory (DFT) and MacroModel Conformational Search (MM) for atomic scale simulations to lend critical insight and understanding for the prediction of structures, chemical mechanisms, and reaction energetics for fundamental reactions.

Capabilities

- Screens high-throughput reaction and catalyst automatically for prediction of reactivity and selectivity, including additional energy and solvation corrections
- Computes rates, barriers, and ML descriptors automatically during post processing
- Identifies lowest energy starting structures with conformational sampling using MacroModel (OPLS4)
- Optimizes geometries and energies ab initio 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

Associated Products: Jaguar, MacroModel



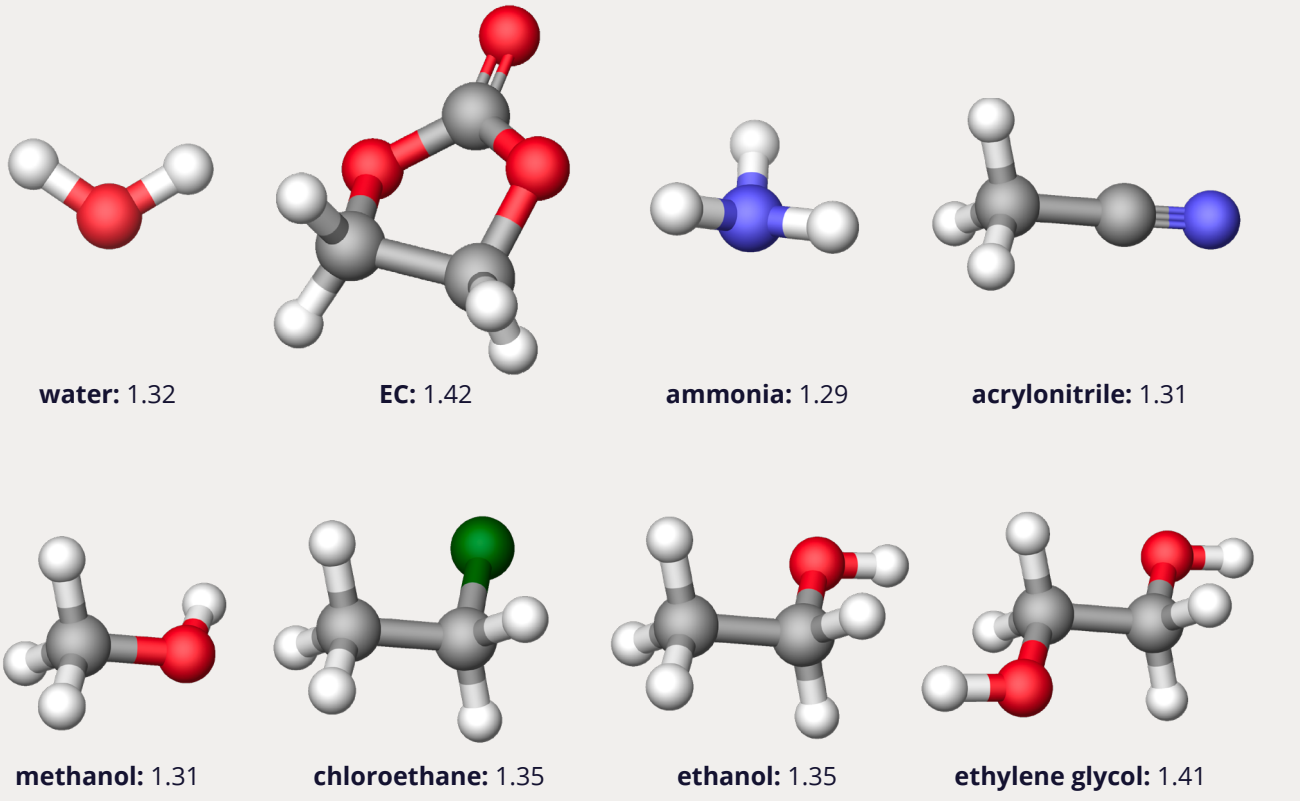
MS Dielectric

MS Dielectric runs both Jaguar Density Functional Theory (DFT) and Desmond Molecular Dynamics (MD) calculations to obtain dielectric properties such as refractive index, electric polarizability, static and complex dielectric constants and dielectric loss function. With an input of a single molecule, all the following system building, simulations, and analysis are performed automatically, creating a single step workflow for dielectric property.

Capabilities

- Computes dielectric properties of molecular materials with combined QM & MD workflows
- 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

AutoTS

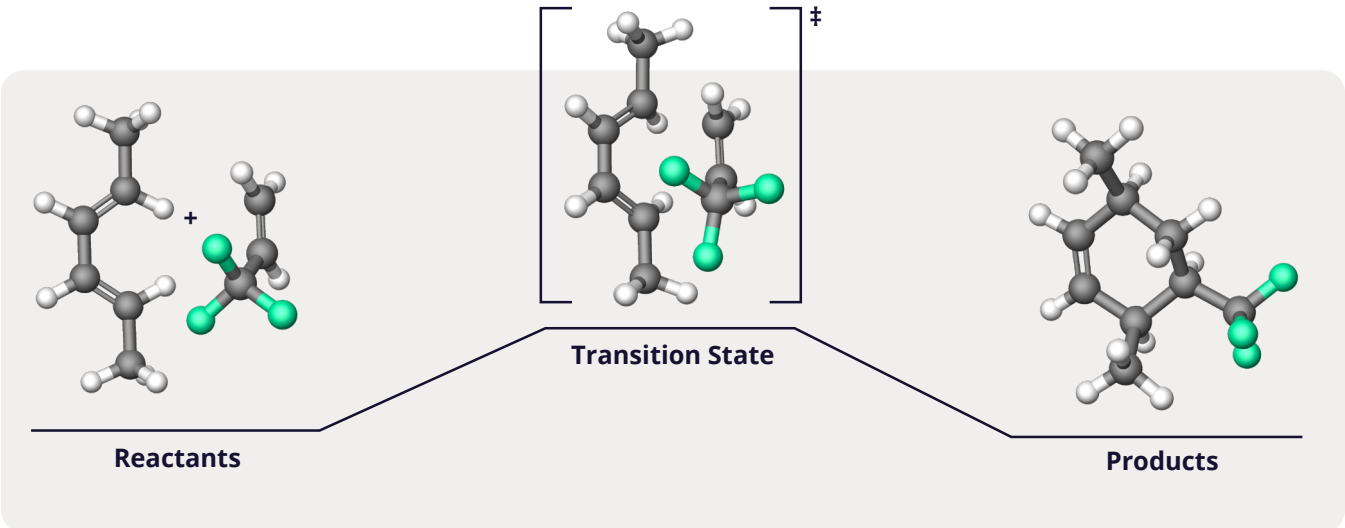
Locating a transition state is necessary for computing the activation energy of a reaction, and thereby the reaction rate. Transition states are essential in many materials science applications: predicting reactivity, understanding reaction mechanisms, designing and optimizing catalysts, predicting outcomes of various competing reactions and more. Locating a transition state is unique to computation — meaning that the transition state cannot be "found" in the lab.

AutoTS is an automated workflow to find transition states, particularly for elementary 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 transition state (TS) between the reactant and product molecules with an automated workflow
- 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 a conformational search on reactants, products, and transition states, outputting statistically averaged reaction energetics

Associated Products: Jaguar, MacroModel



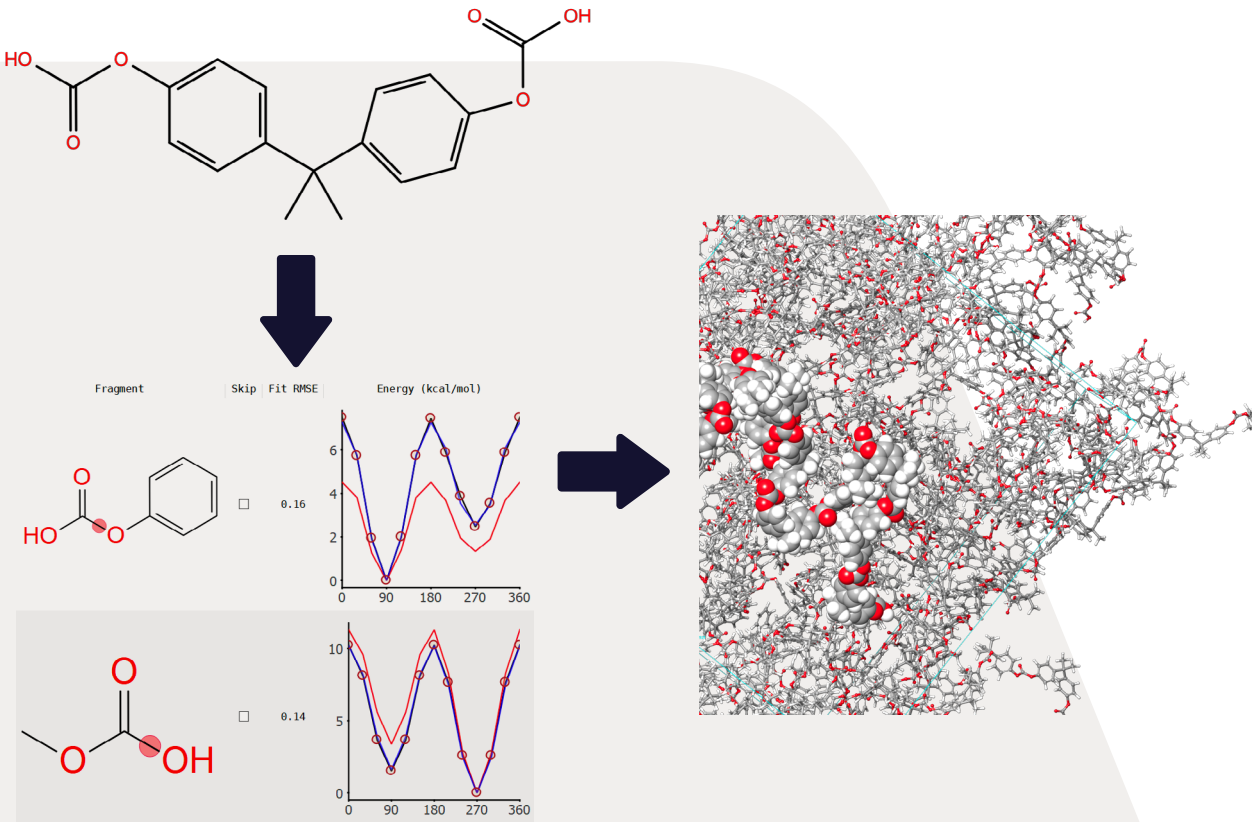
Force Field Builder

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 in OPLS4 force field for previously undefined bond dihedrals
- Visualizes forcefield torsion energy profile compared to QM profile

Associated Products: Jaguar, MacroModel



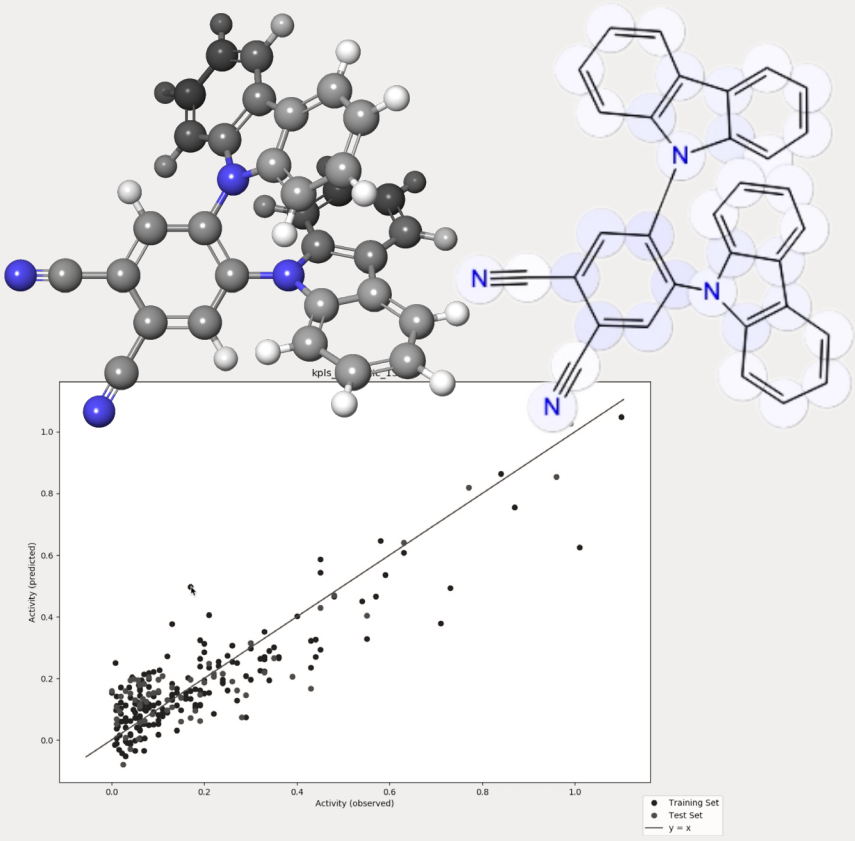
Machine Learning

AutoQSAR

AutoQSAR facilitates the automated creation and application of QSPR machine learning models following a best practices workflow. This best practices workflow includes generation of descriptors, feature selection, creation of a large number of models from exhaustive combinations of descriptors and multiple machine learning methods, and these QSPR models are ranked based on performance. Predictions can then be made from a top ranked QSPR model or from a consensus of the top scoring 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

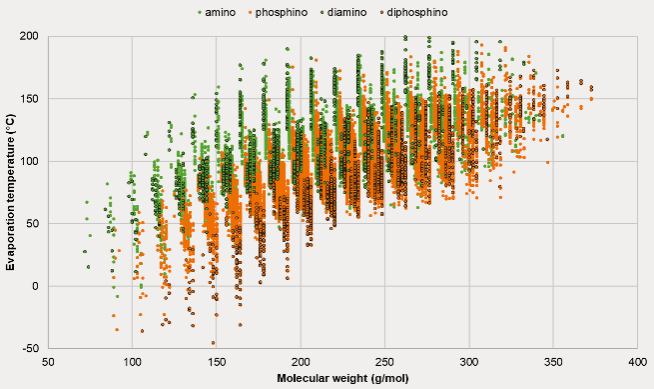


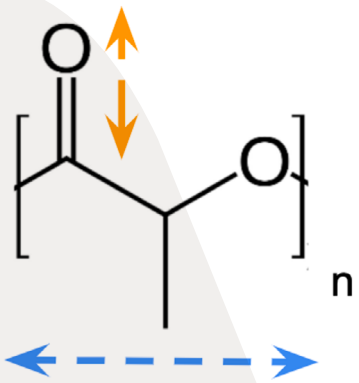
MS Informatics

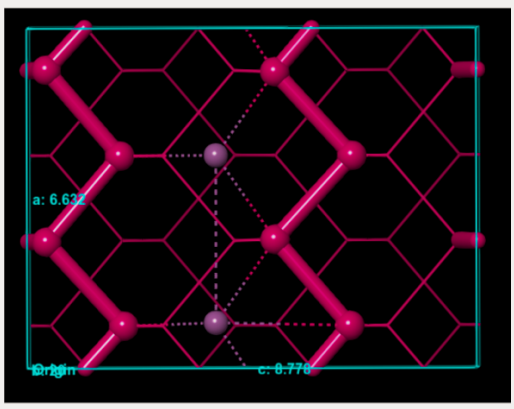
MS Informatics provides machine learning and featurization tools for organic / organometallic molecular materials, polymers, and inorganic periodic solid materials to assist informatics-oriented materials research for building high quality machine learning models.

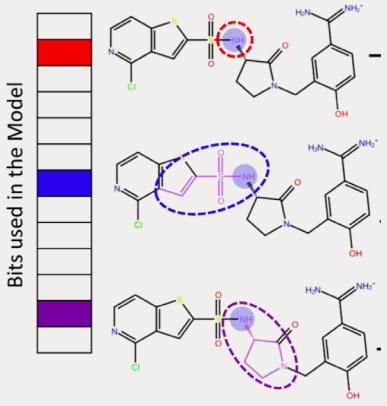
Capabilities

- 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









Scientific and Technical Support

Training resources designed for novice and experts users

Vast educational materials and training courses to make you an expert.

Expert technical and scientific support included

Self-help, email, and face-to-face from industry-leading scientific and technical support.

Cross-platform support for Linux, Windows, Mac, and cloud-based solutions

Designed to work within your computer environment.

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

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