Schrödinger

Schrödinger:
for Academics

Schrödinger

Pioneering Digital Chemistry

30+ years of innovation

Over 850 employees worldwide; >40% Ph.D.

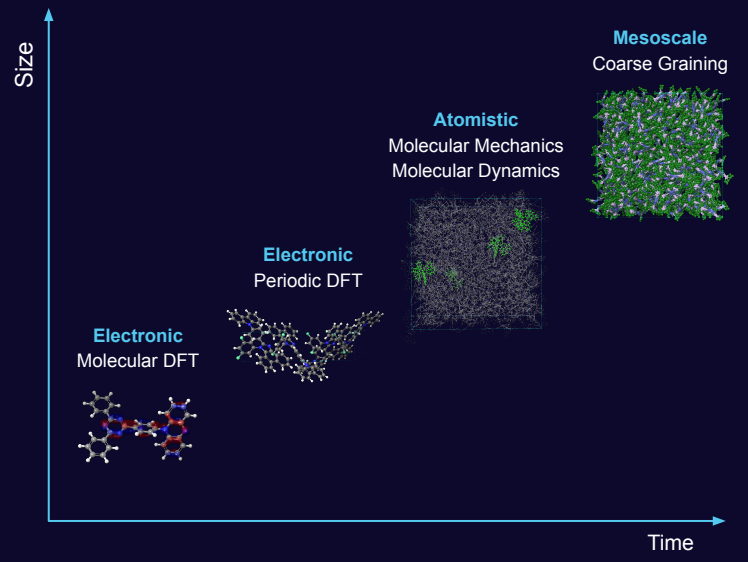
>50% of employees dedicated to R&D

~1,785 customers worldwide

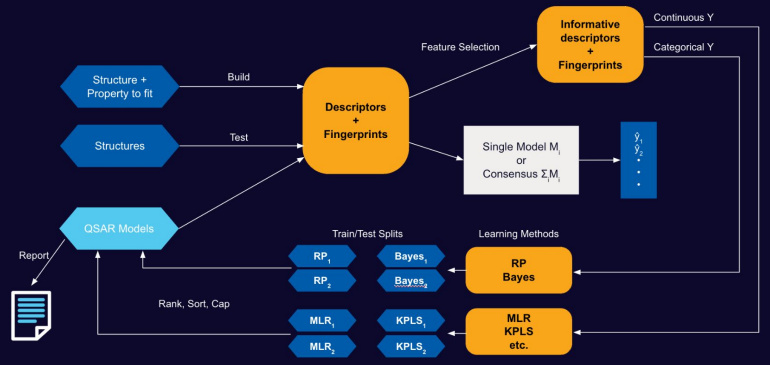
Pipeline of 25+ collaborative and proprietary programs

Digital chemistry strategy built on three pillars

Physics-based modeling



Machine learning



Collaborative informatics

How to work with Schrödinger

Research

Lab License

- Use industry-grade tools for academic research
- A la carte products to meet the specific needs of the research group
- Flexible licensing

Department License

- Use industry-grade tools for academic research
- A la carte products to meet the specific needs of the department
- Flexible licensing

Site License

- Enable both research and education at scale across an entire institution
- All standard products included
- Wide-scale access to education materials

Education

Teaching with Schrödinger

- Incorporate computational chemistry and biology tools in the classroom
- Pre-made lesson plans and hands-on exercises
- Web-based access. No hardware or software needed

Online Certification Courses

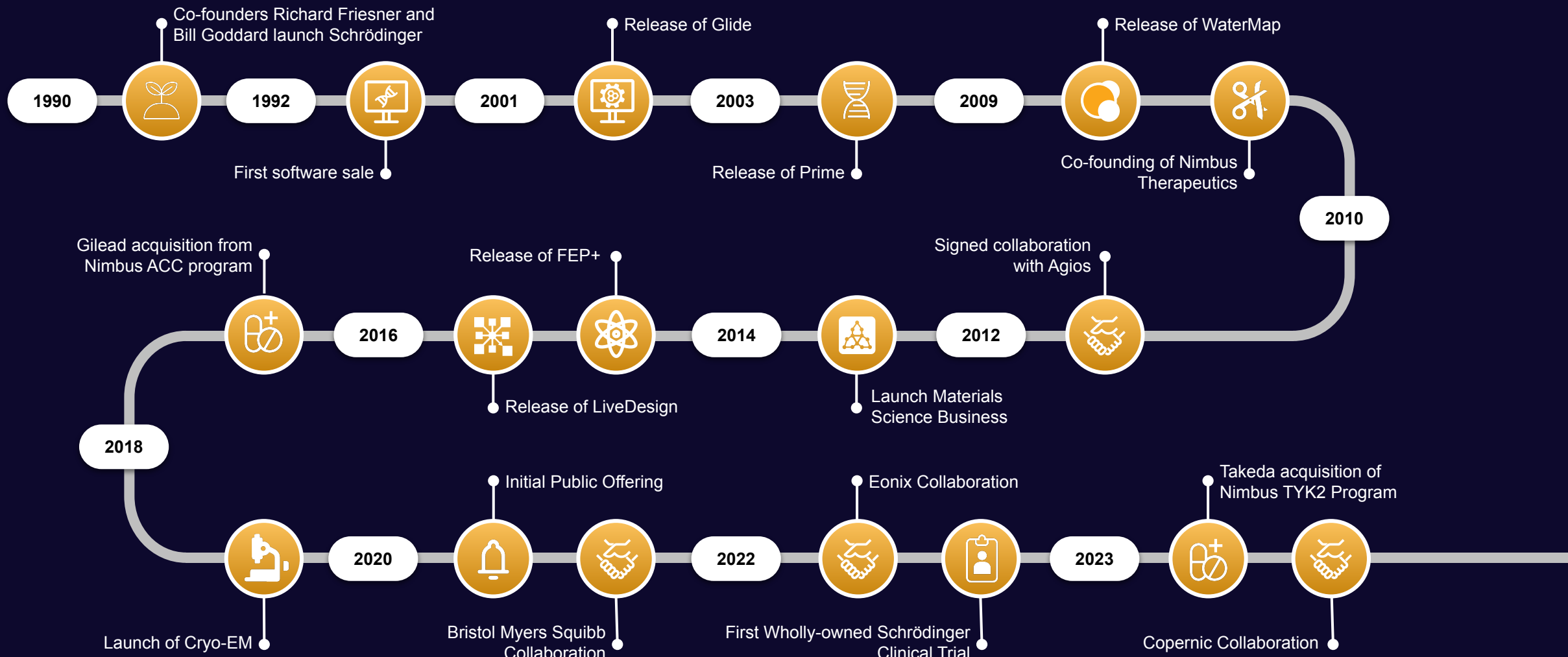
- Hands-on, asynchronous courses ranging from beginner to advanced
- Course material prepared by molecular modeling experts
- Web-based access. No hardware or software needed

Introduction to Schrödinger

MISSION

To improve human health and quality of life by transforming the way new medicines and materials are discovered through advanced computational methods

30+ year history of innovation



A predict-first approach

Traditional materials design

- Manual materials design
- Candidate materials synthesized and tested over **weeks**

Materials selection or purchase

Candidate synthesis and purification

Property testing

!

Candidate materials may not meet requirements

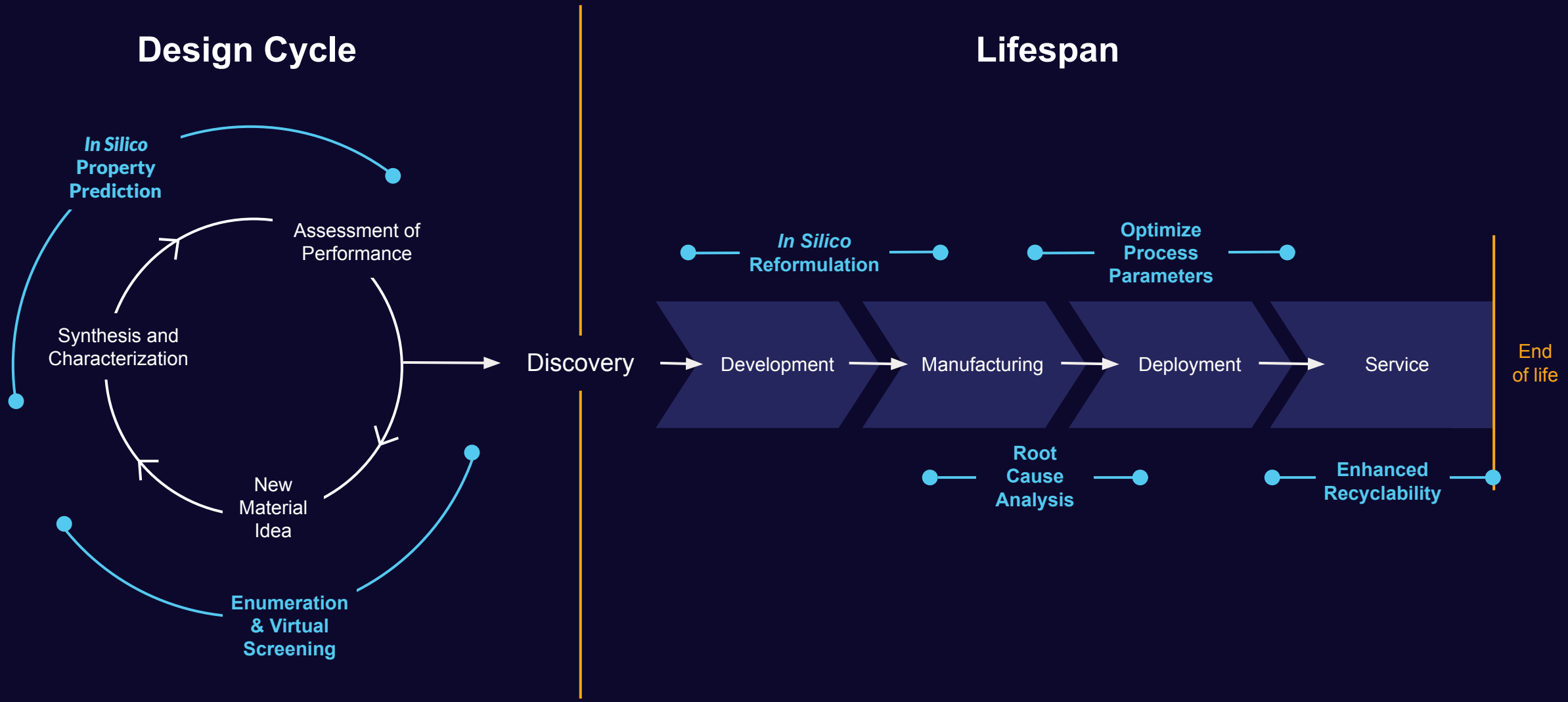
Schrödinger digital chemistry platform

- 100Ks of materials tested computationally
- Candidate materials identified digitally over **days**

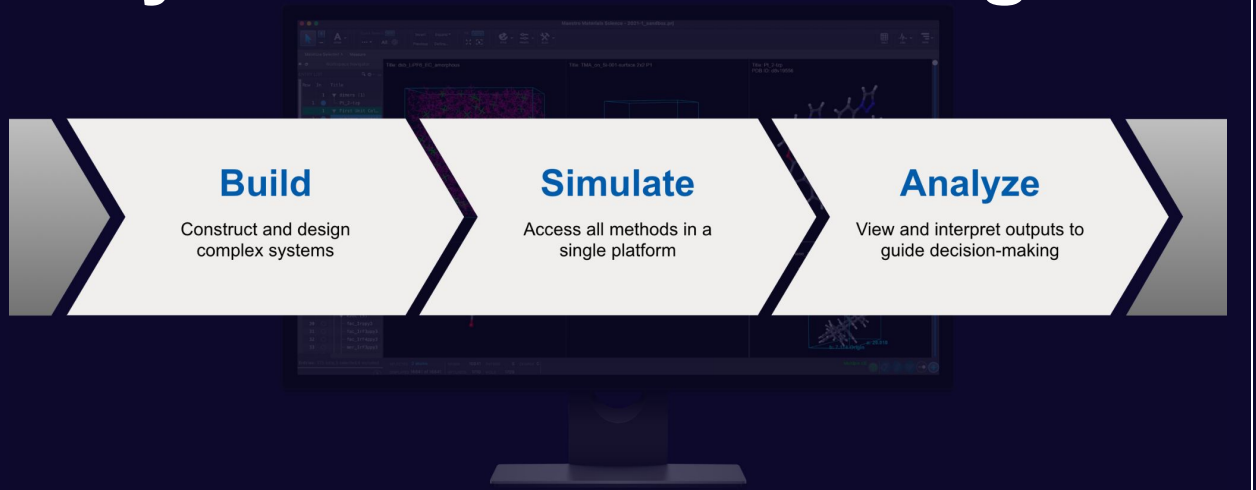
Model building → **Simulations** → **Property predictions** → **Analysis and screen** → ✓

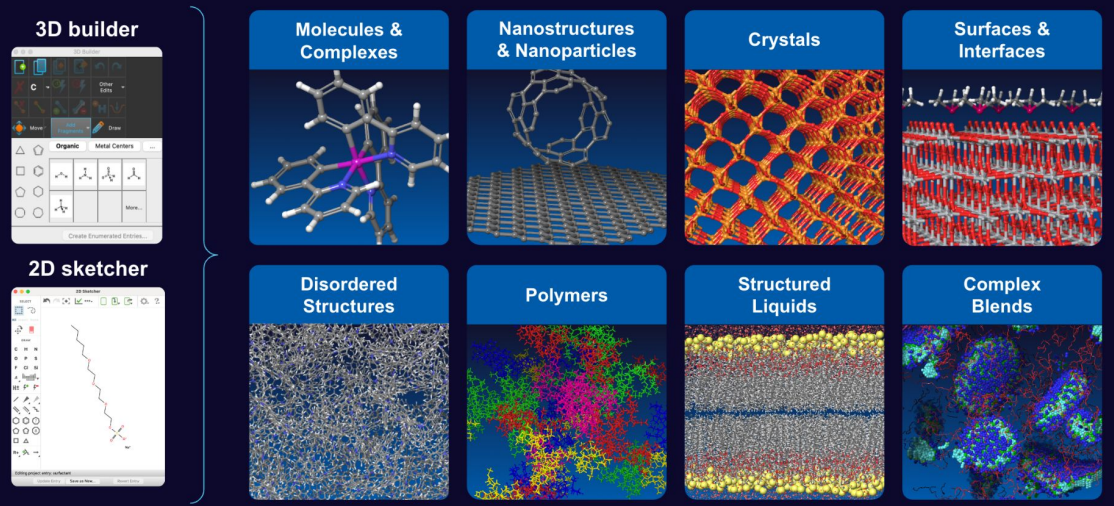
Best performing candidate materials with **optimal property profile**

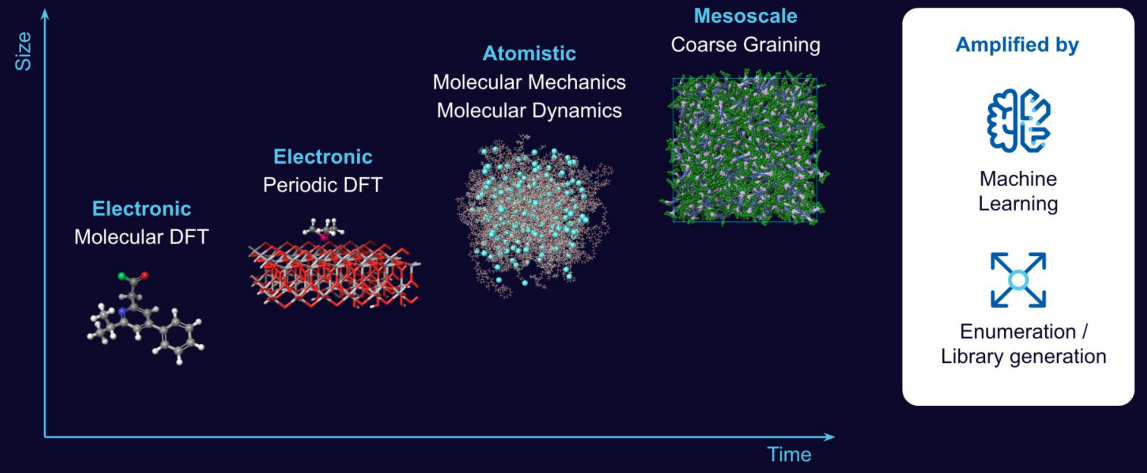
Modeling impact on materials design

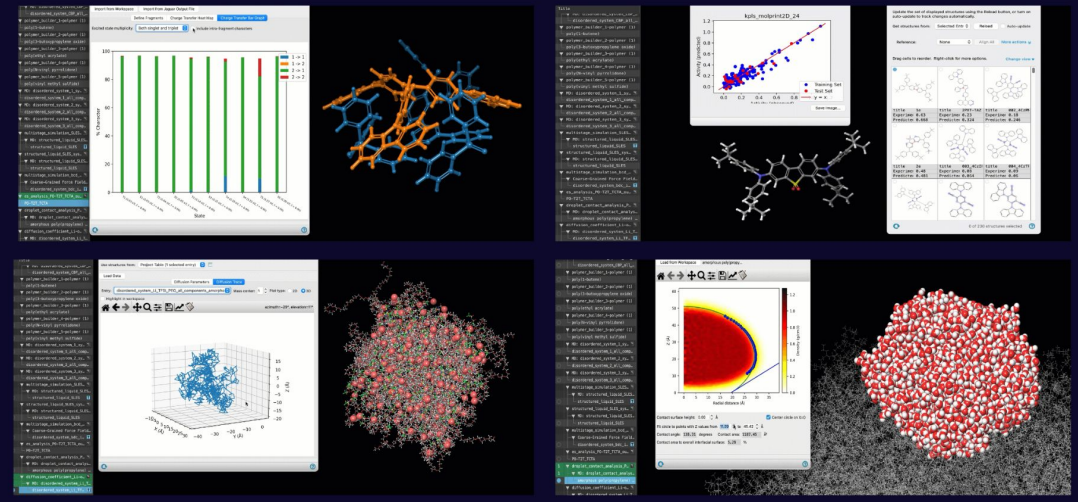


Physics-based modeling

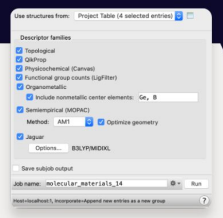








Machine learning

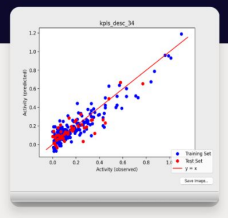


Featurize

Generate extensive descriptors for all classes of materials

Build Models

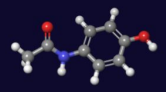
HPC-supported, automated model-building



Predict

Use top model or consensus prediction on unseen systems

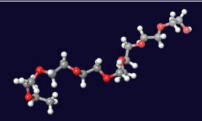
Capabilities for: small molecules, organometallics, polymers, periodic inorganics, and formulations



Small molecules

- Physiochemical, topographical descriptors
- Binary fingerprints (RDKit, Canvas)
- Graph-based convolution neural networks

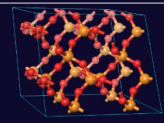
Physics-based descriptors:
- Quantum mechanics
- Auto Reaction Workflow



Polymers

- Taking into account connections between repeat units
- RDKit fingerprints + customized descriptors

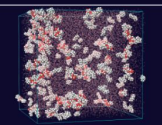
Physics-based descriptors:
- Molecular dynamics
- Quantum mechanics



Periodic inorganic solids

- Element
- Lattice structure
- Oxidation state
- Intercalation descriptors
- 3D SOAP (with PCA)

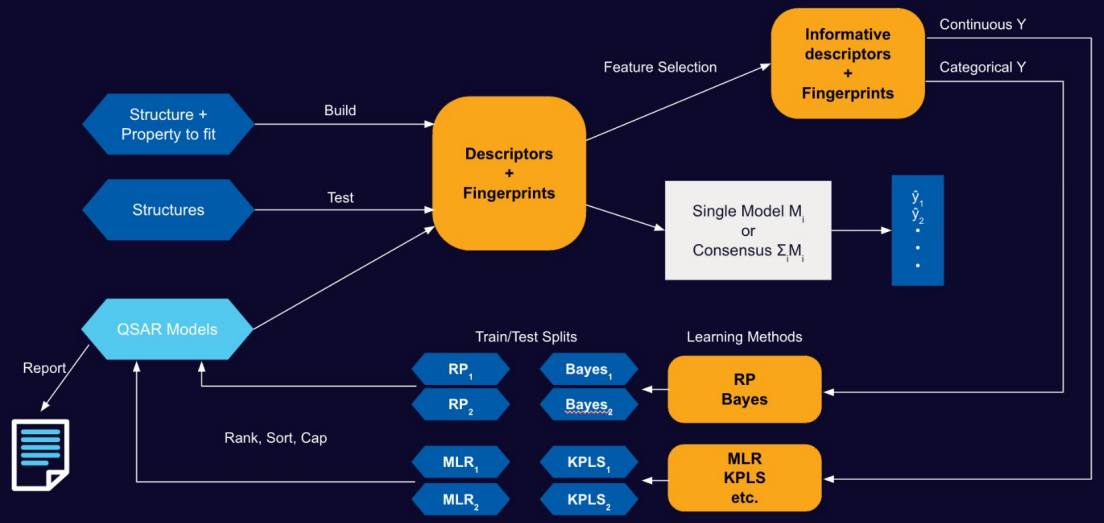
Physics-based descriptors:
- Periodic quantum mechanics



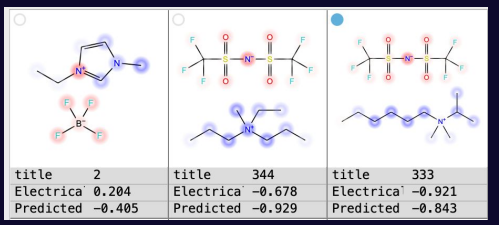
Formulations and mixtures

- Composition
- Chemistry of the components
- Experimental/processing conditions

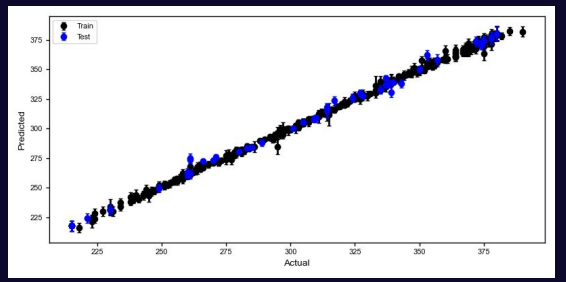
Physics-based descriptors:
- Molecular dynamics

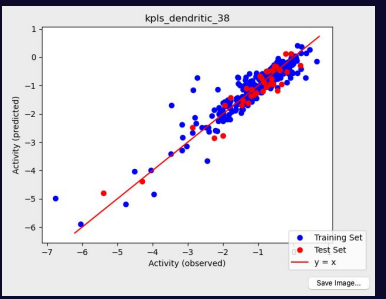


Model Code	Score	S.D.	R^2	RMSE	Q^2	Q^2 MW (Null
kpls_dendritic_38	0.8590	0.3468	0.8584	0.3451	0.9036	-0.0071
kpls_linear_38	0.8319	0.3664	0.8415	0.3770	0.8849	-0.0071
kpls_linear_40	0.8277	0.4017	0.8216	0.3384	0.8400	0.0146
kpls_dendritic_40	0.8159	0.4099	0.8142	0.3912	0.7862	0.0146
kpls_linear_23	0.8039	0.4215	0.8030	0.4084	0.7662	0.0185
kpls_dendritic_23	0.7941	0.4329	0.7921	0.4143	0.7592	0.0185
kpls_radial_21	0.7907	0.4468	0.7836	0.3907	0.7218	-0.0164
kpls_radial_22	0.7833	0.4213	0.8015	0.4255	0.7829	0.0192
kpls_radial_34	0.7805	0.4554	0.7710	0.3895	0.7850	0.0250
kpls_linear_5	0.7793	0.4492	0.7753	0.4219	0.7535	-0.0130



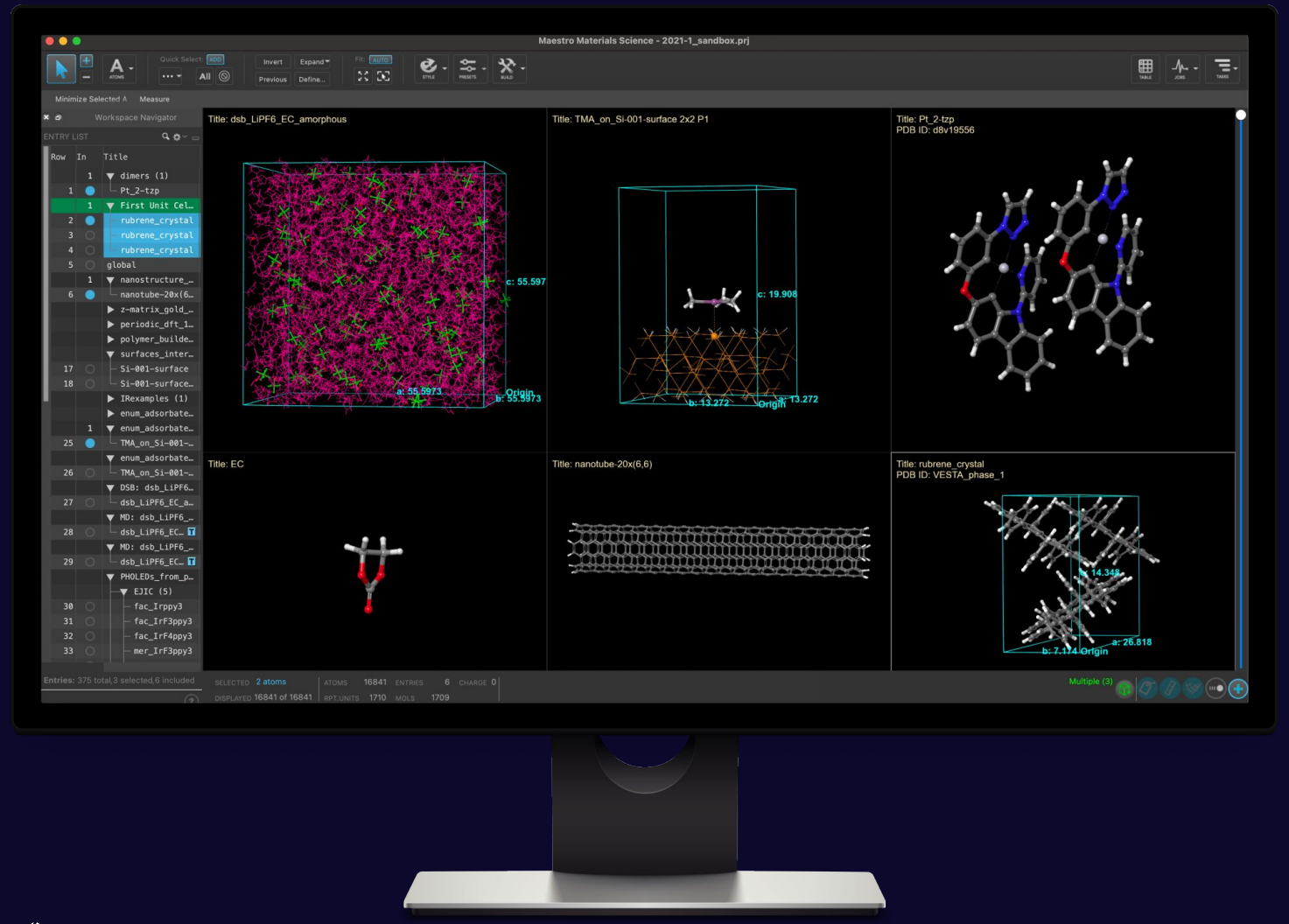
title	2	title	344	title	333
Electrica	0.204	Electrica	-0.678	Electrica	-0.921
Predicted	-0.405	Predicted	-0.929	Predicted	-0.843





User-friendly GUI and comprehensive API

MS Maestro



Python API

Comprehensive API for programmatic interaction with Schrödinger software

```
➜  ~ export SCHRODINGER=/opt/schrodinger/suites2024-1

➜  ~ $SCHRODINGER/run periodic_dft_gui_dir/qe2mae.py -h
usage: $SCHRODINGER/run periodic_dft_gui_dir/qe2mae.py
       [-h] [-last_only] input_file

Converter script from Quantum ESPRESSO output file to Maestro structure
file. Copyright Schrodinger, LLC. All rights reserved.

positional arguments:
  input_file  Quantum ESPRESSO output file (.out, .save.qegz).

optional arguments:
  -h, -help   Show this help message and exit.
  -last_only  Save only last structure. (default: False)
➜  ~
```

Products

Jaguar

A high-performance quantum chemistry software program leveraging the pseudospectral approximation method

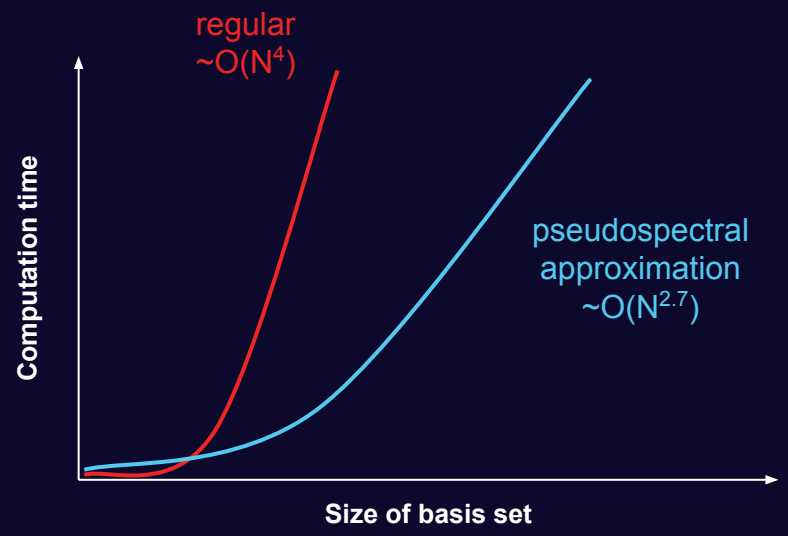
Key capabilities:

- Extensive coverage of functionals, basis sets, and properties, see Jaguar Data Sheet
- Geometry optimization, transition state search, thermochemical properties, implicit solvation, spectra prediction, and more
- Automated solutions: pKa prediction, conformationally averaged VCD and ECD spectroscopy, tautomer generation and ranking, heat of formation, etc.
- Publication-quality 3D surfaces: molecular orbitals, electrostatic potential projected on isodensity, spin density, non-covalent interactions, etc.

Visit webpage

Speed-up (hybrid DFT):

- Single points: ~ 2-4x
- Geometry optimizations: ~ 2-3x
- Second derivatives: ~ 2x
- TD-DFT: ~ 10x

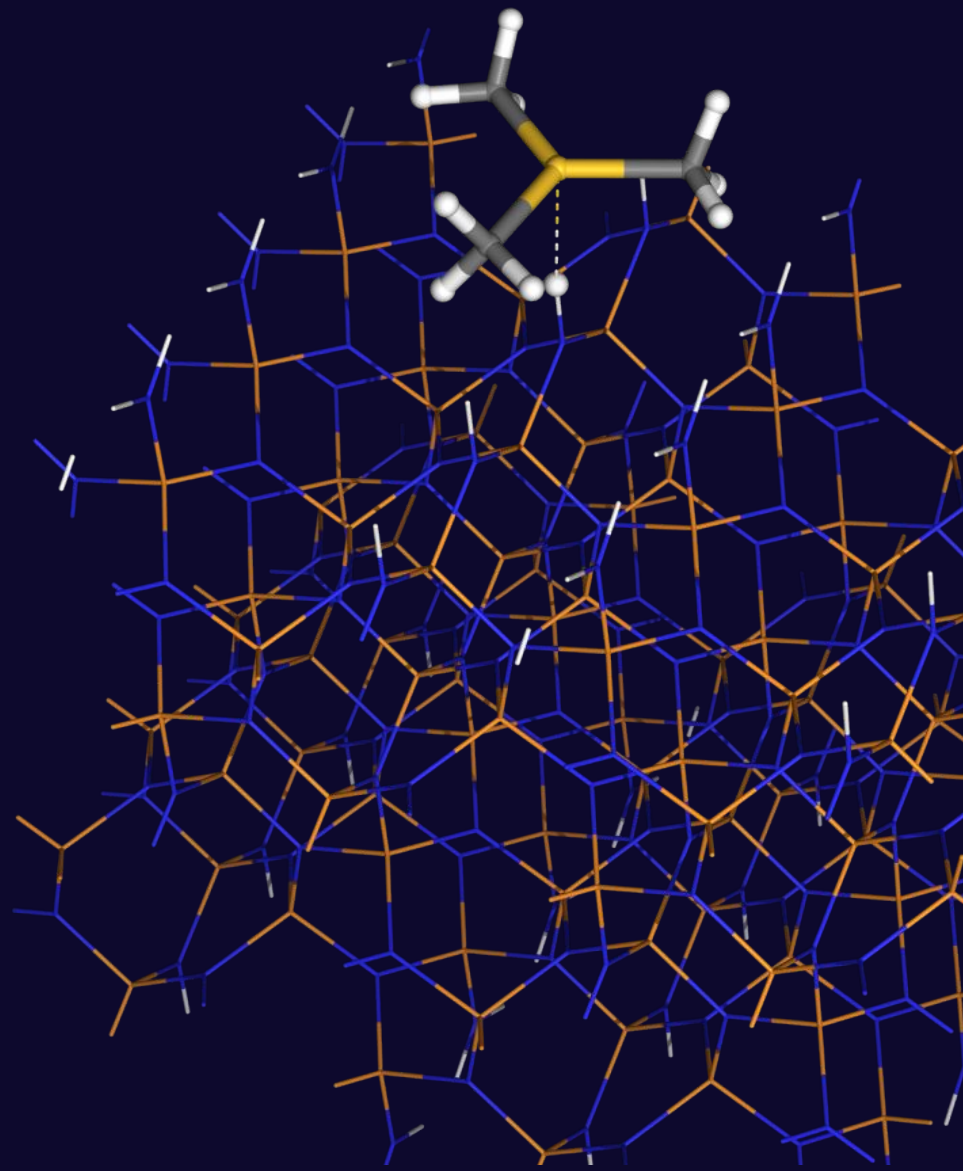


Schrödinger

Plot adapted: https://www2.lbl.gov/Science-Articles/Archive/CSD-quantum-chemistry.html
Latest Jaguar Review: J. Chem. Phys. 161, 052502 (2024)

Quantum ESPRESSO

Automated solutions, including builders and analysis tools for performing periodic DFT calculations



Key capabilities:

- Predictions for bulk, surface, and interface properties
- Support Ultrasoft (US), Norm-Conserving (NC) and Projector Augmented Wave (PAW) pseudopotentials
- Perform structural optimization and ab initio molecular dynamics
- Simulate transition states and minimum energy paths with nudged elastic band (NEB) method
- Model linear response properties within Density Functional Perturbation theory (DFPT)
- Predict spectroscopic properties

Visit webpage

Desmond

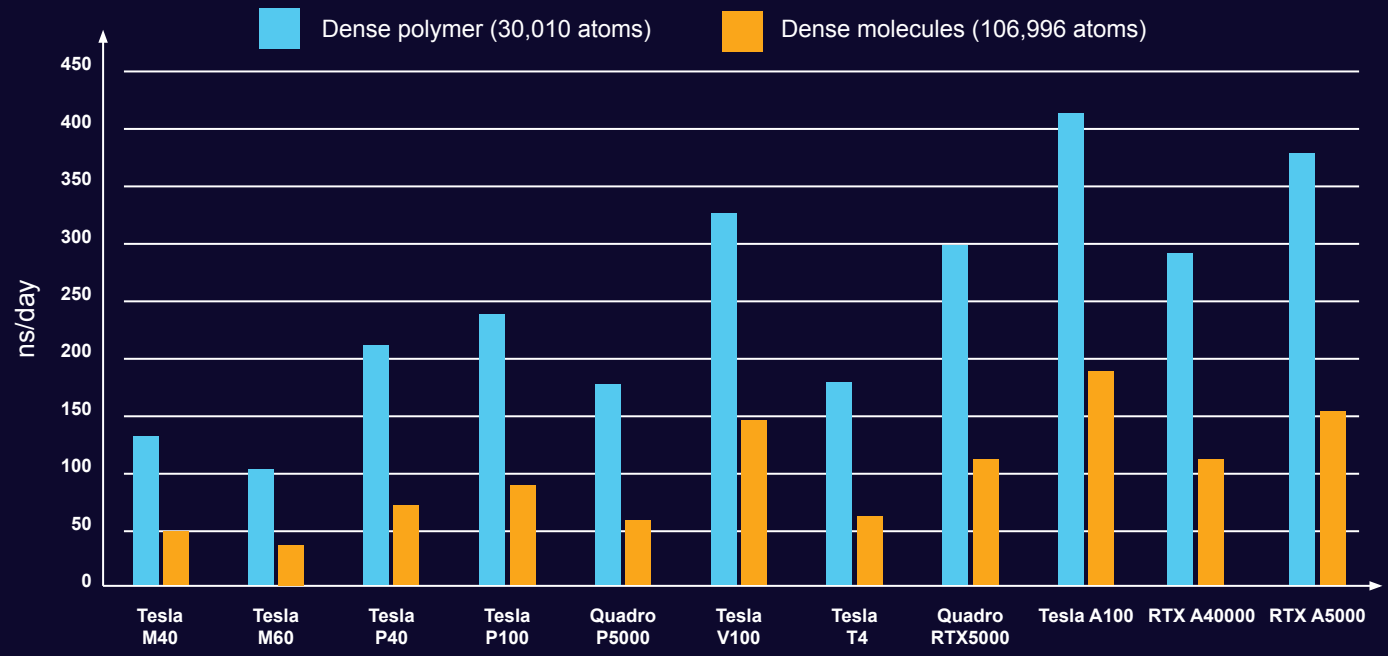
High-performance molecular dynamics (MD) engine providing high scalability, throughput, and scientific accuracy

Key capabilities:

- GPU
- OPLS and coarse-grained force fields
- Enhanced sampling including replica exchange
- Extensively validated for materials science applications

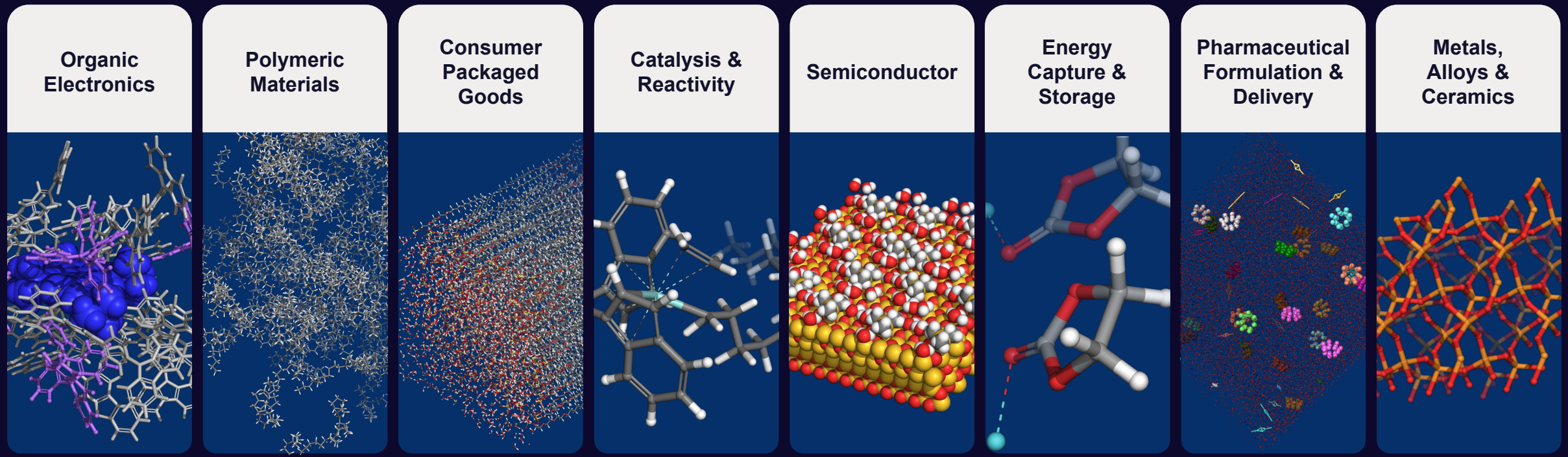
Visit webpage

Desmond Molecular Dynamics Performance



Application Areas and Select Capabilities

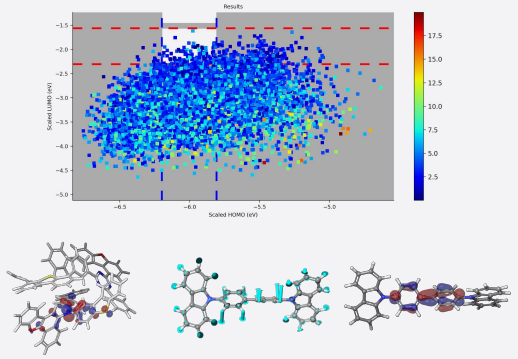
Solutions for all applications



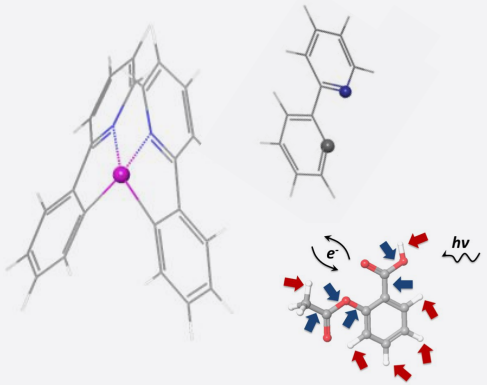
Tailored solutions that reduce cost, reduce risk, shorten timelines

Organic electronics: select capabilities

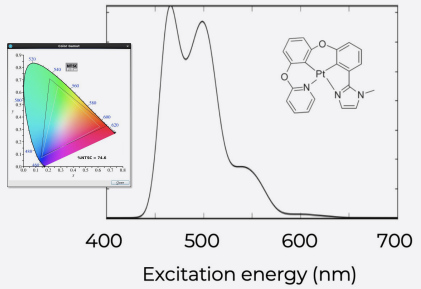
Optoelectronic properties



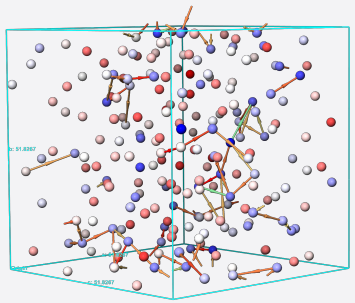
Chemical stability



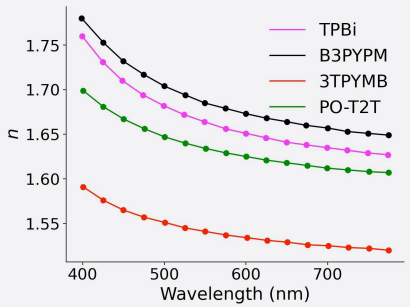
Absorption and emission spectra



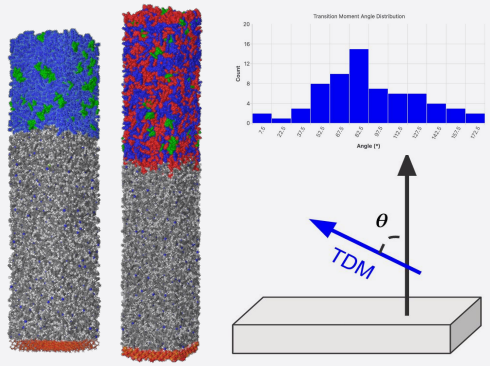
Charge mobility



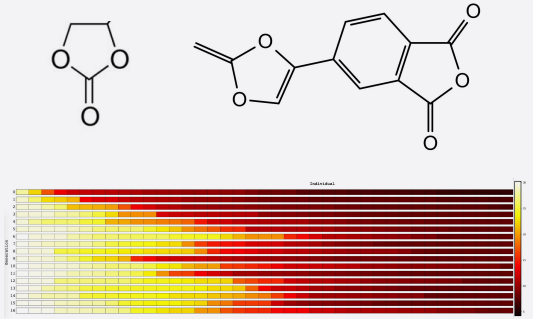
Dielectric properties



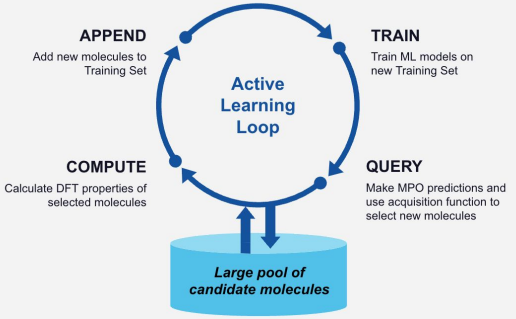
Molecular deposition



Genetic optimization

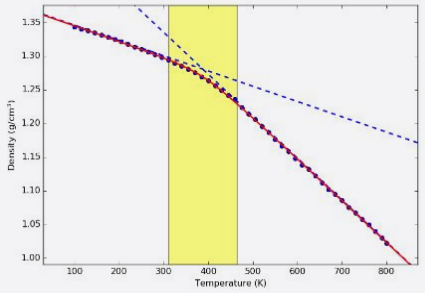


Active learning

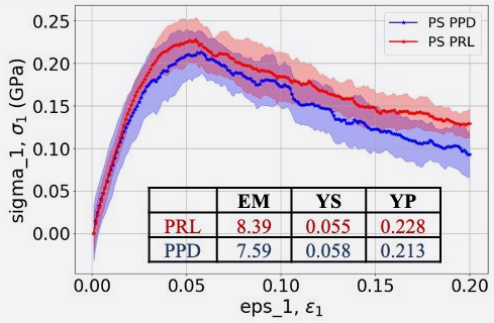


Polymeric materials: select capabilities

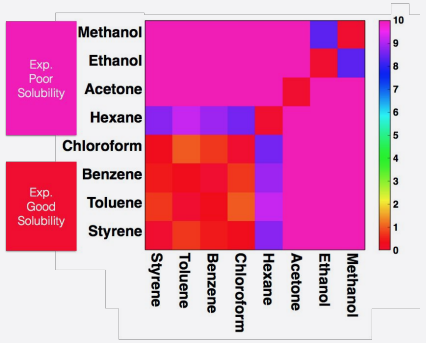
Glass transition temperature



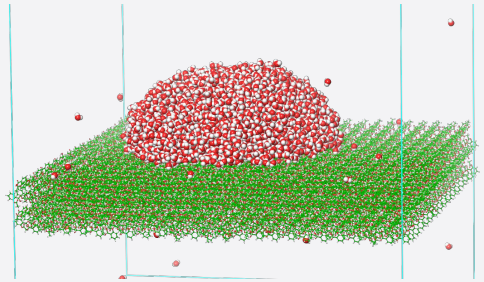
Mechanical response



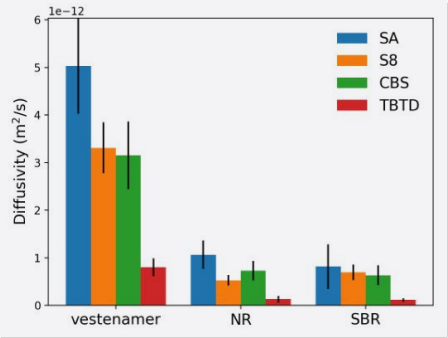
Miscibility and solubility



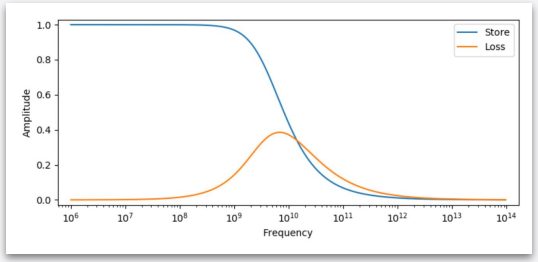
Contact angle



Diffusivity

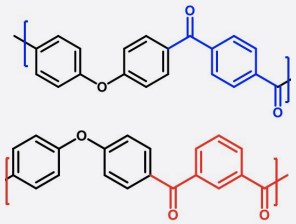


Dielectric properties



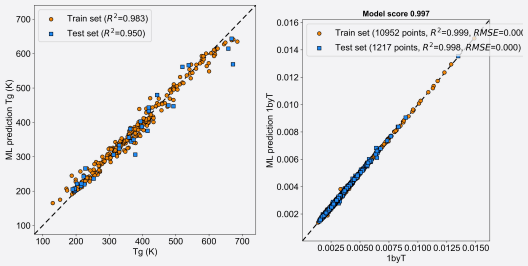
Bond dissociation energy

Bond Dissociation Energy (kcal/mol)	
Ether	Ketone
85.67 ± 1.91	98.86 ± 3.26
77.76 ± 1.04	90.36 ± 1.02



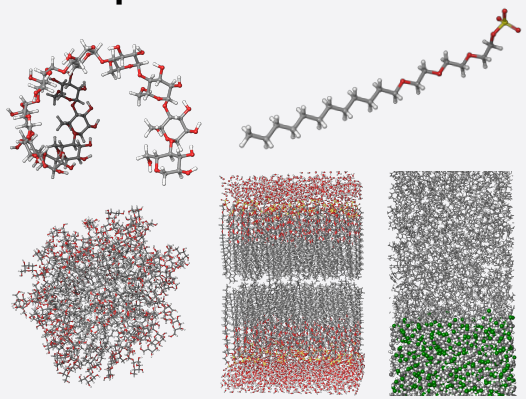
Croshaw, C. et al. *Polymer degradation and stability* **2022**, *200*, 109968.

ML property prediction



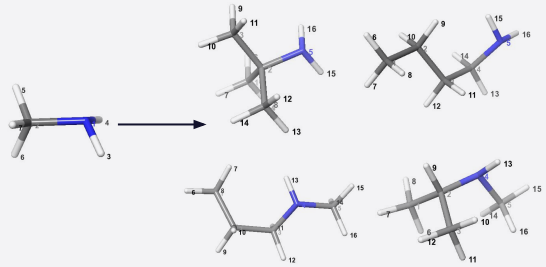
Consumer packaged goods: select capabilities

Complex structure builders

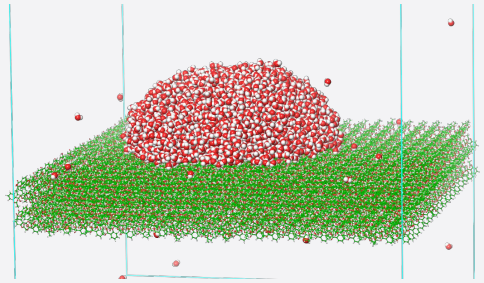


Predict degradation products

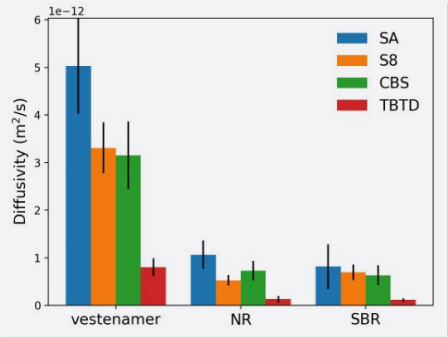
Reactivity



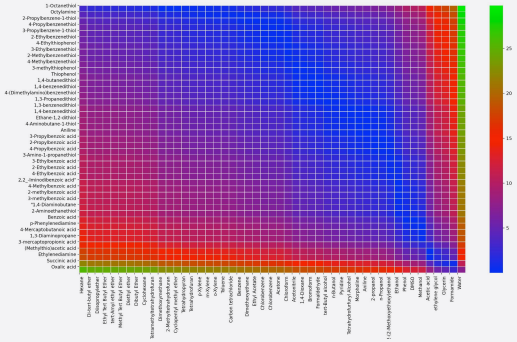
Contact angle



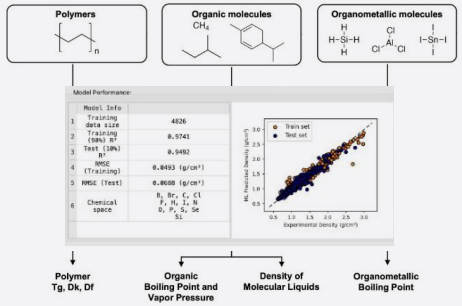
Diffusivity



Miscibility and solubility

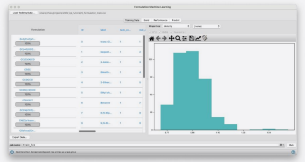


ML property prediction

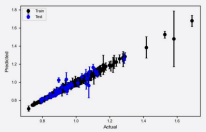


ML for formulations

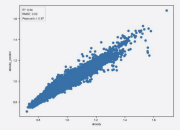
Training: 431 examples of N=1 to N=5 component solvents



Test R^2 of 0.87 achieved in predicting density

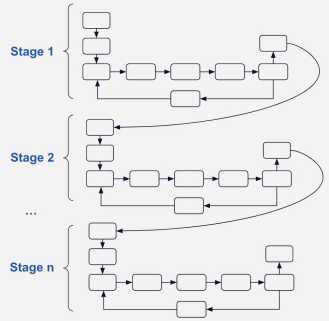


Model generalizes to ~30K formulations with R^2 of 0.94

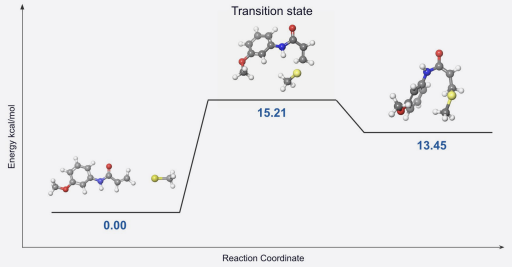


Catalysis and reactivity: select capabilities

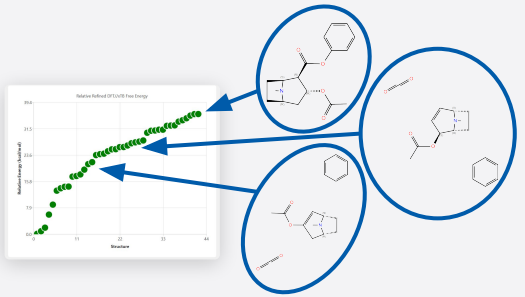
Multistage quantum mechanical solutions



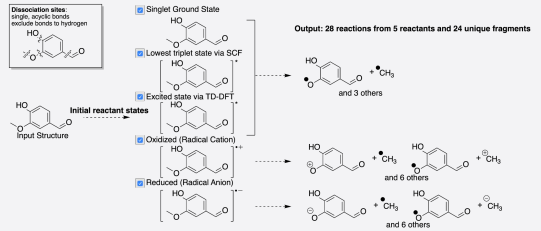
Automated transition state searching



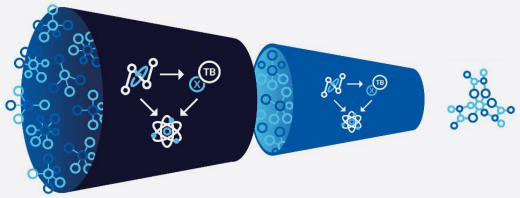
Degradation products prediction



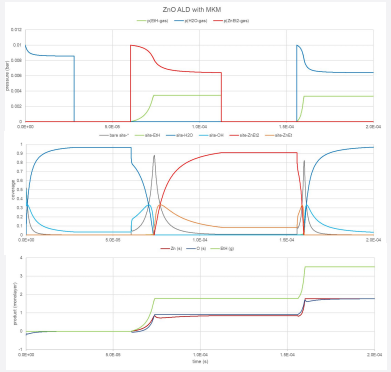
Bond dissociation energies



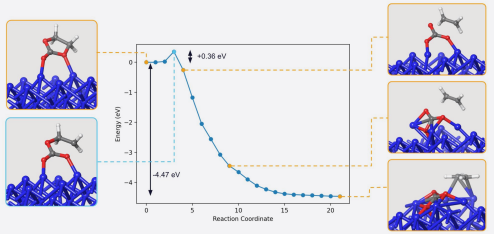
Molecular catalyst design



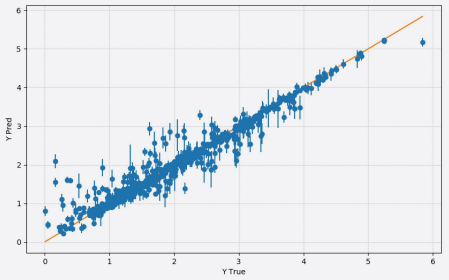
Microkinetic modeling



Surface reactivity

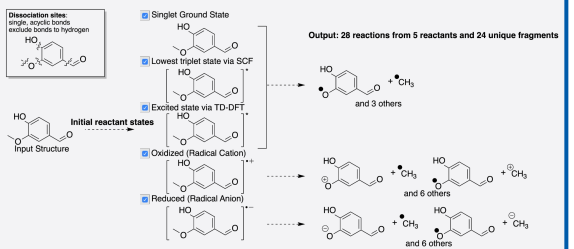


Cheminformatics for catalyst design

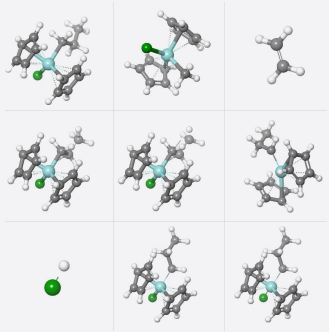


Semiconductor: select capabilities

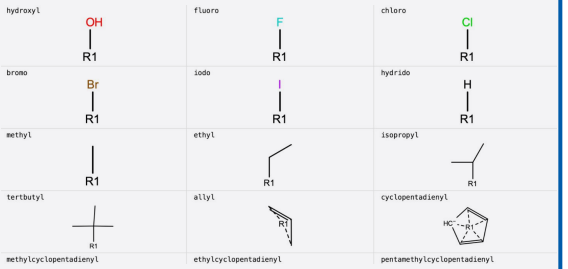
Thermal stability: homolytic bond dissociation



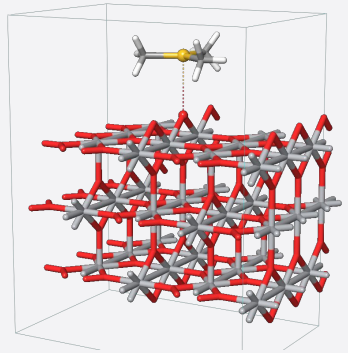
Thermal stability: beta-hydride elimination



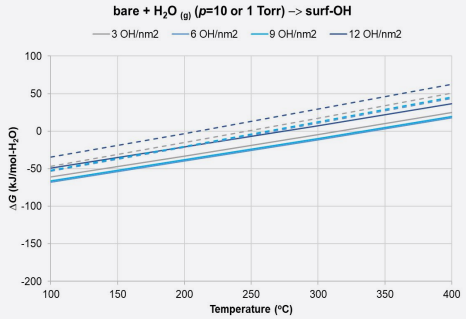
Ligand exchange stability



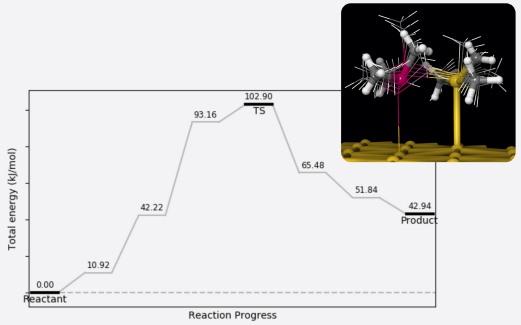
Thermodynamics of adsorption



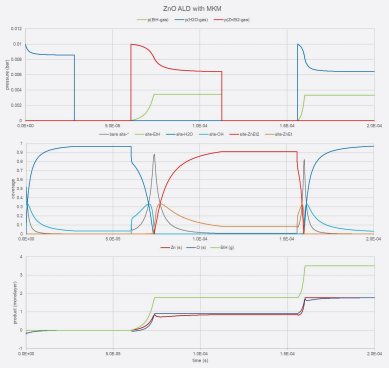
Reactivity towards deposition or etching



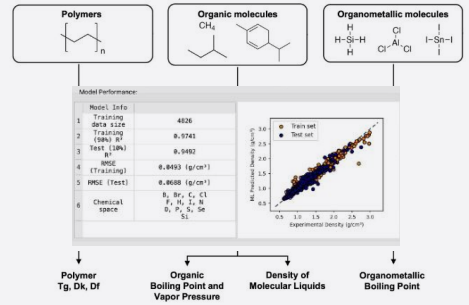
Kinetics of surface reactions



Microkinetic modeling

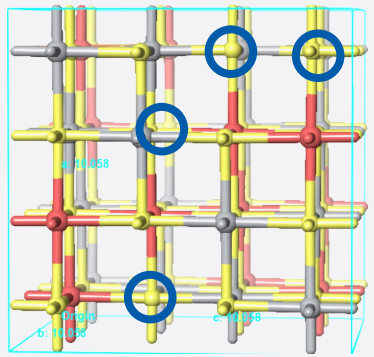


Evaporation/sublimation temperature

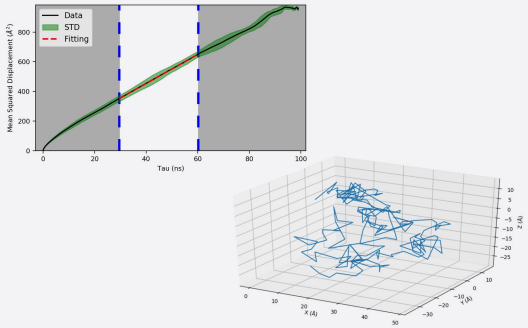


Energy capture and storage: select capabilities

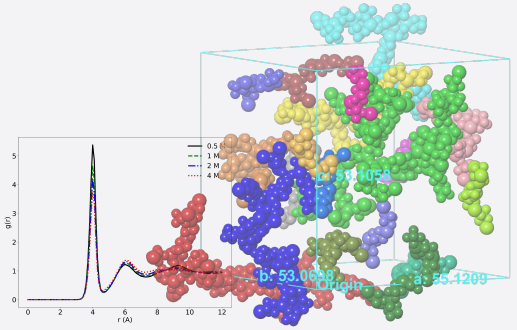
Electrode properties



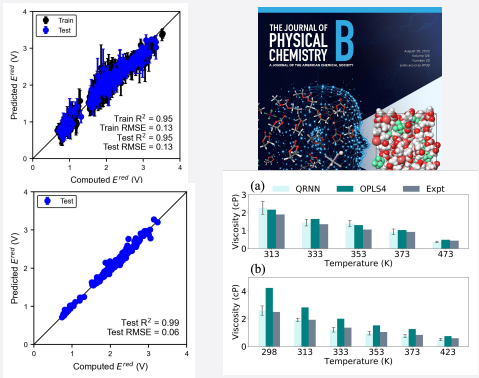
Transport properties: diffusion and viscosity



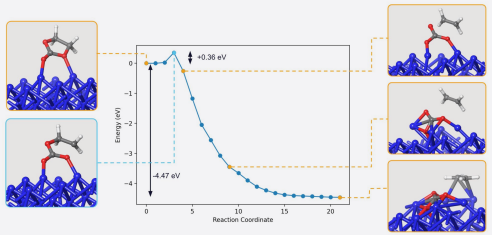
Electrolute structure analysis



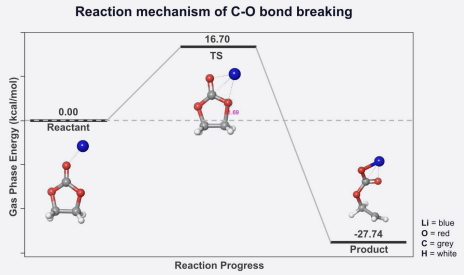
ML models and ML-FF



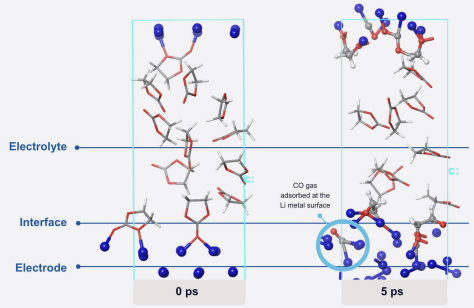
Surface reactivity



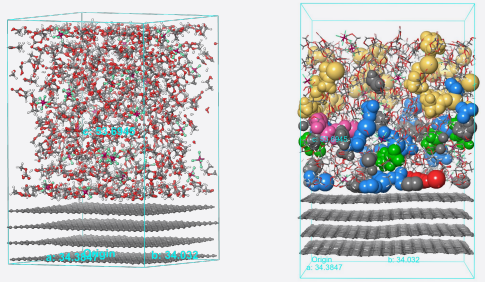
Small molecule reactivity



Electrolyte degradation

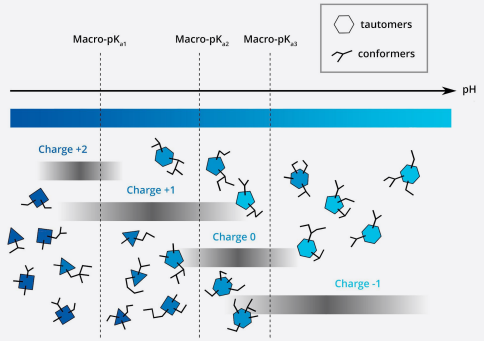


Solid electrolyte interphase morphology

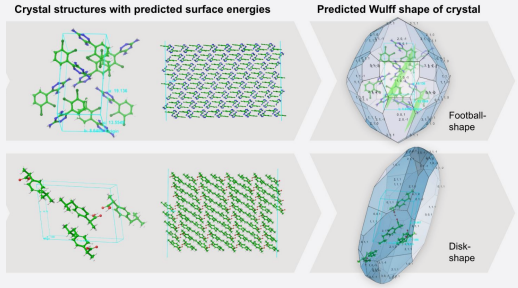


Pharmaceutical formulations: select capabilities

pKa

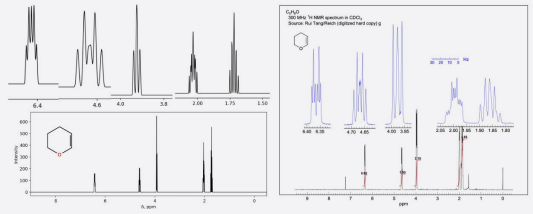


Crystal morphology

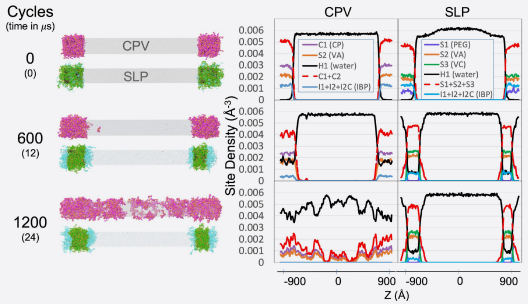


Degradation products prediction

Spectroscopy e.g. VCD, NMR, UV-Vis

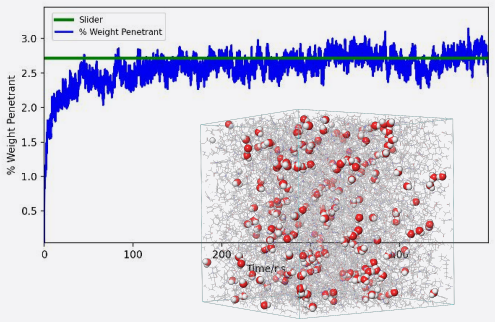


ASD formulation

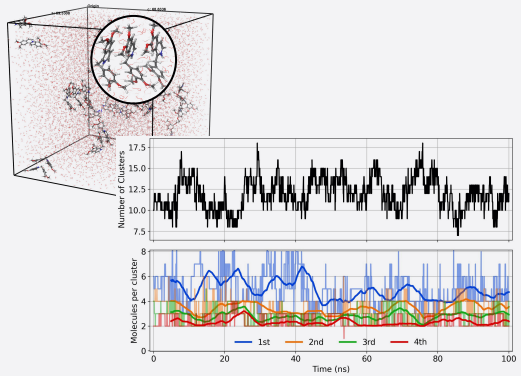


Afzal et al. Mol. Pharm. 2021, 18 3999

Moisture sorption

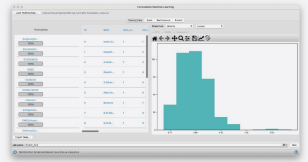


API aggregation

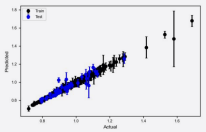


ML for formulations

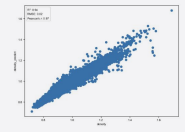
Training: 431 examples of N=1 to N=5 component solvents



Test R^2 of 0.87 achieved in predicting density



Model generalizes to ~30K formulations with R^2 of 0.94



Capabilities: organic electronics

Efficiency & Performance

- Light emission / absorption / colors
  - Spectrum peaks and shapes (FWHM)
  - Multispectra analysis from individual RGB characteristics
- Molecular electronic properties
  - Representative orbital energies (HOMO/LUMO)
  - Transition dipole moment
  - Excited state energy level with oscillator strengths
  - Energy transfer from optically excited states
- Charge transport and recombination
  - Charge reorganization energy
  - Charge carrier mobility
  - Excited-state charge transfer and localization characteristics
- Outcoupling efficiency
  - Dielectric constant/loss
  - Molecular film orientation

Stability & Lifetime

- Bond dissociation energy for the ground and the excited states
- Chemical reaction analysis for potential degradation pathways

Processing & Film Morphology

- Thermophysical properties
  - Glass transition temperature
  - Coefficient of thermal expansion
- Process-oriented film morphology prediction
  - Molecular deposition
  - Solvent evaporation
  - Solvent uptake
- Mechanical properties
  - Elastic constants
  - Stress-strain curve
- Solubility/miscibility
- Thermal conductivity

Materials Design & Discovery

- Chemical enumeration and library generation
  - Digitization for chemistry and data
  - R-group / ligand enumeration
- Machine learning for electronic materials
  - Automated machine learning algorithms for model building and validation
  - Machine learning for materials formulations
  - Active learning for materials screening
- Creation and management of new generative models for designing novel electronic materials (services)

Enterprise Informatics

- Enterprise platform for OLED materials R&D
  - Management of materials information
  - Automated molecular simulations
  - Cheminformatics and machine learning
  - Management of OLED device data with links to materials information

Capabilities: thin film processing

Precursor Design & Development

- Structure and properties of precursor compounds
  - Metal-ligand bonding
  - Molecular volume
  - Surface coverage / steric demand of ligands
- Precursor chemistry
  - Customizable, built-in library of hundreds of ligands for ALD/CVD processes including monodentate, bidentate (κ^2), and haptic (η^5) ligands
  - Automated & flexible enumeration over ligands to generate libraries of candidate precursors
  - High-throughput quantum mechanical calculations for virtual screening of candidate precursors
  - Reactivity with respect to deposition or etch of target film (oxide, nitride, metal etc)
- Thermal stability assessment
  - Homolytic bond dissociation
  - β-hydride elimination
  - Synthetic stability with respect to ligand exchange
- Machine learning prediction for physical properties of organometallic compounds
  - Volatility (evaporation or sublimation temperature at a given pressure)

Surface Chemistry Analysis

- Thermodynamics of molecular adsorption onto surfaces
  - Automated generation of adsorption geometries
  - High-throughput predictions of adsorption free energies
- Surface reactivity
  - Thermochemistry of deposition & etching processes
  - Temperature windows or crossover temperatures for competing surface processing
  - Chemical reactivity of plasma components at surface
  - Reaction kinetics via activation energies
- Time evolution of surface coverages during ALD cycles via microkinetic modeling
  - Saturation time
  - Growth per cycle
  - Sticking coefficient

Data Management & Collaboration

- Enterprise solution for managing database and molecular ideation
  - Web-based, chemically-aware informatics platform
  - Management of both experimental and computed materials data
  - Support for collaboration across geographies and departments
- Built-in machine learning and cheminformatics solutions for property predictions and smart search/screening

Capabilities: battery materials

Electrode Materials

- System builders (crystals, slabs and interfaces, series of point defects)
- Surface energy
- Equilibrium lattice constants
- Density of states and band gaps
- Mechanical properties (elastic constants / bulk moduli)
- Dielectric constants
- Ion migration in bulk structures with nudged elastic band (NEB) simulations
- Intercalation potential
- Defect formation energies with corrections for charged defects
- Equation of state predictions
- Effective screening medium

Electrolyte Materials and Formulations

- Model builders (molecules, elemental and functional group enumeration, polymers)
- Machine learning cheminformatics for single- and multi-component systems
- Machine learning force fields for electrolyte systems (services)
- Molecular properties
  - Orbital energies and redox potentials
  - Atomic charges and polarizability
  - Density profile
- Liquid or polymer electrolyte properties
  - Viscosity
  - Dielectric constants and loss
  - Glass transition temperature (Tg) and coefficient of thermal expansion
  - Diffusivity and ionic conductivity
  - Solubility parameters
  - Mechanical properties (e.g. stress-strain curves)
  - Clustering and aggregation
  - Electrolyte-ion coordination
  - Radial distribution function (RDF) and structure factor

Electrolyte Reactivity and Stability

- Degradation
  - Bond dissociation energies
  - Prediction of decomposition products
- Reaction mechanism elucidation (molecules)
  - Energy landscape for reactants, intermediates, and products
  - Automated transition state search

Solid Electrolyte Interphase

- Solid-electrolyte interphase simulator for constructing SEI models
  - Reaction-template-based molecular dynamics simulation with multiple reaction components
- Ab initio MD (AIMD) for the study of early stage SEI formation mechanisms
- Reaction mechanism elucidation (surfaces)
  - Energy landscape for reactants, intermediates, and products
  - Transition state search (NEB)

Capabilities: petrochemical

Heterogeneous Catalysis, Surface Chemistry

- Builders and enumeration (crystals, slabs, adsorbates)
- Reaction mechanism elucidation
  - Thermodynamics and kinetics: reactants, intermediates, and products
  - Automated transition state search
- Microkinetic modeling
- Machine learning cheminformatics

Energy Capture and Storage

- Battery materials
  - Electrode materials
  - Electrolyte materials
  - Solid-electrolyte interphase
- Electrolyte stability and reactivity towards electrode materials
- Materials for carbon capture
- Hydrogen and methanol storage and delivery

Homogeneous Catalysis, Reactivity, Degradation

- Builders and enumeration
- DFT, xTB, ML potentials
- Conformational search
- Degradation
  - Bond dissociation energies
  - Prediction of decomposition products
- Reaction mechanism elucidation
  - Multistage quantum mechanics: reactants, intermediates, and products
  - Automated transition state search (AutoTS)
- Automated physics-based and ML cheminformatics-based catalyst design:
  - Selectivity (chemo-, regio-, enantioselectivity)
  - Activity (TOF)

Spectroscopy / Characterization

- pKa
- VCD, IR/Raman/UV-Vis
- NMR (solution-state, solid-state)

Polymers, Additives, Rubbers, Lubricants, Emulsions

- Builders and enumeration (polymers, surfactants, micelles, multicomponent mixtures, interfaces)
- Bio-based polymers (e.g. PET)
- All-atom molecular dynamics simulation
- Coarse-grained simulation
- Phase behavior
- Compatibility and dispersion
- Properties of polymers/soft matter/mixtures:
  - Diffusivity and viscosity
  - Miscibility and solubility
  - Glass transition temperature
  - Coefficient of thermal expansion
  - Dielectric properties
  - Stress-strain curves
  - Clustering/aggregation
  - Interaction energies
- Thermoset modeling (cross-linking)
- Catalysts for polymerization reactions
- Machine learning cheminformatics for polymers and formulations

Capabilities: pharmaceutical formulation and delivery

Characterization

- pKa
- Powder X-ray diffraction (XRPD)
- Crystal morphology
- Density of crystalline or amorphous phases

Catalysis, Reactivity, Degradation

- API degradation
  - Bond dissociation energies
  - Prediction of decomposition products
- Reaction mechanism profile
  - Thermodynamics (ΔG,ΔH) and kinetics (E_a): reactants, products, intermediates, transition states
  - Automated transition state search
- Automated catalyst design
- Machine learning models for catalysis
- Conformational search

Spectroscopy

- VCD
- Solution-state NMR
- Solid-state NMR
- IR/Raman
- UV-Vis

Crystal Structure Prediction (CSP)

- CSP for de-risking (services)
- CSP for scaffold design (services)
- CSP software (coming soon)

Formulations and Delivery

- Machine learning models for formulations
- System builders (mixtures, polymers, surfactants, lipids, etc.)
- Solubility of amorphous and crystalline API
- API aggregation
- Glass transition temperature
- Mechanical properties
- Wettability (contact angle)
- Separation during solvent removal (evaporation)
- API encapsulation in cyclodextrin, etc.
- Excipient selection and ASD formulation
  - API solubility and LogP in excipient
  - Solubility parameters
  - API — excipient mixing enthalpy
  - ASD separation and dissolution
  - Protein/biologics excipients selection
- Hygroscopicity (moisture sorption) in
  - Amorphous solid dispersions
  - APIs
  - Tablet coatings
- Solution viscosity
- Protein/polymer interactions
- Lipid nanoparticles
- mRNA formulations (services)
- Liposomes

Capabilities: aerospace and defense

Polymers, Composites and Formulations

- Builders and enumeration (homopolymers, block copolymers, semicrystalline polymers, ladder polymers, carbohydrates/biopolymers, multicomponent mixtures, interfaces, formulations)
- Methods
  - All-atom molecular dynamics simulation (OPLS force field)
  - Coarse-grained simulation
    - Martini force field (database parameters)
    - Dissipative particle dynamics (DPD), automated particulation and force field parameterization
- Physics-based prediction of:
  - Glass transition temperature (Tg)
  - Coefficient of thermal expansion (CTE)
  - Mechanical response (e.g. stress-strain, elastic constants)
  - Penetrant loading (water, solvent; function of relative humidity and/or temperature)
  - Evaporation
  - Diffusivity and migration
  - Conformational statistics
  - Dielectric properties (e.g. refractive index, Abbe number, static dielectric constant, complex permittivity)
  - Wettability (contact angle)
  - Interaction energy at interface
  - Clustering/aggregation/additive binding
  - Viscosity
  - Thermal conductivity
  - Surface tension
  - Miscibility (solubility parameters), solubility of additives/contaminants
  - Enzyme degradation

Reactivity and Catalysis

- Cross-linking
  - Realistic curing simulations
  - Prediction of gel point
- Polymer and molecular degradation
  - Bond dissociation energies
  - Prediction of decomposition products
- High energy materials
- Reaction mechanism elucidation
  - Energy landscape for reactants, intermediates, and products
  - Automated transition state search
- Automated catalyst design
- Polymerization reaction barriers

Machine Learning

- Descriptor generation
  - Molecular descriptors
  - Polymer descriptors
  - Formulation descriptors (composition)
- Pre-trained ML models (e.g. dielectric constant, glass transition temperature)
- Automated ML model building

Solid-State Materials

- Builders and enumeration
  - Crystals (pure inorganics, alloys, additives/dopants)
  - Slabs and interfaces
- Physics-based prediction of:
  - Surface energy
  - Equilibrium lattice constants
  - Density of states and band gaps
  - Mechanical properties (elastic constants / bulk moduli)
  - Dielectric constants
  - Ion migration in bulk structures with nudged elastic band (NEB) simulations
  - Intercalation potential
  - Defect formation energies with corrections for charged defects
  - Equation of state predictions
  - Effective screening medium
- Microkinetic modeling
- Reaction mechanism elucidation
  - Energy landscapes
  - Automated transition state search

Capabilities: plastics, elastomers and polymer-based materials

Physics-based Property Estimation

- Builders and enumeration (homopolymers, block copolymers, semicrystalline polymers, ladder polymers, carbohydrates/biopolymers, multicomponent mixtures, interfaces, formulations)
- Methods
  - All-atom molecular dynamics simulation (OPLS force field)
  - Coarse-grained simulation
    - Martini force field (database parameters)
    - Dissipative particle dynamics (DPD), automated particulation and force field parameterization
- Physics-based prediction of:
  - Glass transition temperature (Tg)
  - Coefficient of thermal expansion (CTE)
  - Mechanical response (e.g. stress-strain, elastic constants)
  - Penetrant loading (water, solvent; function of relative humidity and/or temperature)
  - Evaporation
  - Diffusivity and migration
  - Conformational statistics
  - Dielectric properties (e.g. refractive index, Abbe number, static dielectric constant, complex permittivity)
  - Wettability (contact angle)
  - Interaction energy at interface
  - Clustering/aggregation/additive binding
  - Viscosity
  - Thermal conductivity
  - Surface tension
  - Miscibility (solubility parameters), solubility of additives/contaminants (e.g. FEP Solubility)
  - Enzyme degradation

Catalysis, Reactivity and Degradation

- Cross-linking
  - Realistic curing simulations
  - Prediction of gel point
- Polymer degradation
  - Bond dissociation energies
  - Prediction of decomposition products
- Reaction mechanism elucidation
  - Energy landscape for reactants, intermediates, and products
  - Automated transition state search
- Automated catalyst design
- Polymerization reaction barriers

Spectroscopy and Characterization

- Solution-state NMR
- IR/Raman
- UV-Vis
- pKa
- Powder X-ray diffraction (XRPD)
- Density of crystalline or amorphous phases

Machine Learning

- Descriptor generation
  - Molecular descriptors
  - Polymer descriptors (topological fingerprints and structural descriptors)
  - Formulation descriptors (composition)
- Pre-trained ML models (e.g. dielectric constant, dissipation loss, glass transition temperature)
- Automated ML model building for molecules, polymers and formulations

Capabilities: consumer packaged goods

Physics-based Property Estimation

- Builders and enumeration (homopolymers, block copolymers, ladder polymers, carbohydrates, multicomponent mixtures, interfaces, formulations)
- Methods
  - All-atom molecular dynamics simulation (OPLS force field)
  - Coarse-grained simulation
    - Martini force field (database parameters)
    - Dissipative particle dynamics (DPD), automated particulation and force field parameterization
- Physics-based prediction of:
  - Glass transition temperature (Tg)
  - Coefficient of thermal expansion (CTE)
  - Mechanical response (e.g. stress-strain, elastic constants)
  - Penetrant loading (water, solvent; function of relative humidity and/or temperature)
  - Evaporation
  - Diffusivity
  - Migration of contaminants
  - Conformational statistics
  - Wettability (contact angle)
  - Clustering/aggregation
  - Viscosity
  - Thermal conductivity
  - Surface tension
  - Miscibility (solubility parameters), solubility (e.g. FEP Solubility)
  - Electroporation
  - Antimicrobial activity
  - Protein-based biomaterial stability

Catalysis, Reactivity and Degradation

- Cross-linking
  - Realistic curing simulations
  - Prediction of gel point
- Polymer degradation
  - Bond dissociation energies
  - Prediction of decomposition products
- Reaction mechanism elucidation
  - Energy landscape for reactants, intermediates, and products
  - Automated transition state search
- Automated catalyst design

Spectroscopy and Characterization

- VCD
- Solution-state NMR
- Solid-state NMR
- IR/Raman
- UV-Vis
- pKa
- Powder X-ray diffraction (XRPD)
- Crystal morphology
- Density of crystalline or amorphous phases

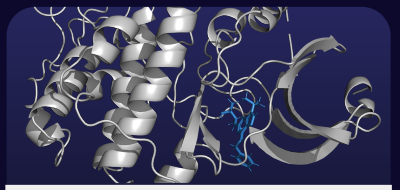
Machine Learning

- Descriptor generation
  - Molecular descriptors
  - Polymer descriptors (topological fingerprints and structural descriptors)
  - Formulation descriptors (composition)
- Pre-trained ML models (e.g. glass transition temperature)
- Automated ML model building for molecules, polymers and formulations

Education

Schrödinger Online Courses

Full suite of online certification courses

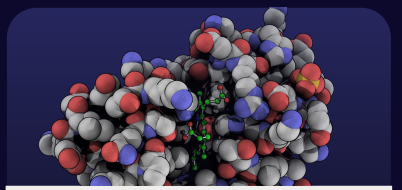


Introduction to Molecular Modeling in Drug Discovery

Protein preparation, ligand docking, collaborative design, and other fundamentals of small molecule drug discovery with Maestro and LiveDesign.

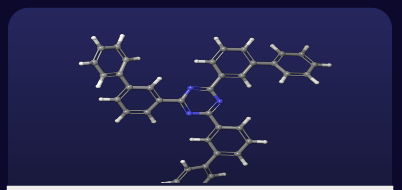
Introduction to Computational Antibody Engineering

Structure-based workflows for assessing and improving the developability, stability, affinity, and 'humanness' of antibody therapeutics with BioLuminate



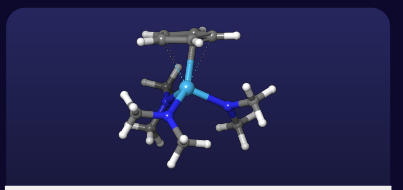
Visualizing Science with PyMOL 3

Unlock the power of molecular movie making in PyMOL with the Visualizing Science with PyMOL 3 Online Certification Course



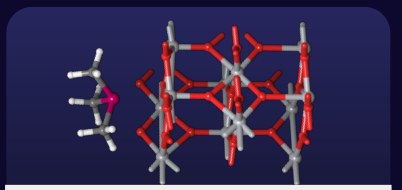
Organic Electronics

Molecular quantum mechanics, all-atom molecular dynamics, and machine learning approaches for studying challenges in OLED design and discovery



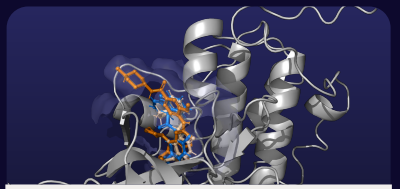
Homogeneous Catalysis and Reactivity

Molecular quantum mechanics and machine learning approaches for studying reactivity and mechanism at the molecular level



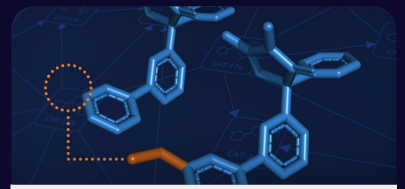
Surface Chemistry

Molecular quantum mechanics, periodic quantum mechanics, and machine learning approaches for studying atomic layer processing and heterogeneous catalysis



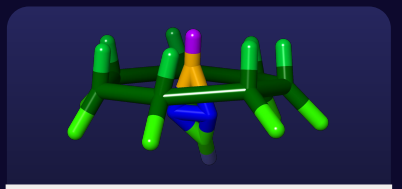
High-Throughput Virtual Screening for Hit Finding and Evaluation

Computational target analysis as well as best practices for both structure-based and ligand-based virtual screening of large ligand libraries



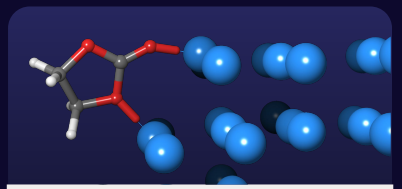
Free Energy Calculations for Drug Design with FEP+

Running, analyzing, and troubleshooting relative binding FEP+ calculations for small molecule lead optimization



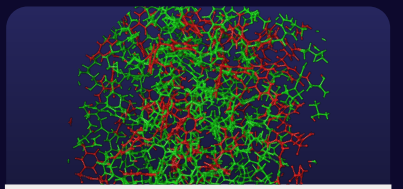
Pharmaceutical Formulations

Molecular and periodic quantum mechanics, all-atom molecular dynamics, and coarse-grained approaches for studying active pharmaceutical ingredients and their formulations



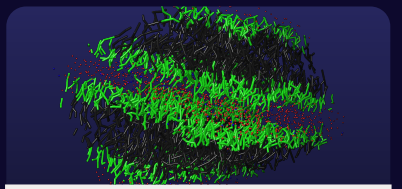
Battery Materials

Molecular and periodic quantum mechanics, all-atom molecular dynamics, and machine learning for studying battery materials and their properties under various conditions



Polymeric Materials

All-atom molecular dynamics and machine learning approaches for studying polymeric materials and their properties under various conditions



Consumer Packaged Goods

All-atom molecular dynamics, coarse-grained, and machine learning approaches for studying materials integral to the formulation of CPG

Organic Electronics

Module 1

Introduction to Materials Modeling

2 hours

Video: Introduction to Materials Modeling & This Online Course

Video Tutorial: Introduction to Materials Science (MS) Maestro

Video: Modeling for Organic Electronics

Module 2

Molecular Quantum Mechanics

7 hours + Comp Time

Video: Introduction to Molecular Quantum Mechanics (mQM)

Tutorials:

- Functionals, Basis Sets and Geometry Optimizations
- R-Group Enumeration
- QM Multistage Workflows
- Optoelectronics
- Organometallic Complexes
- Bond and Ligand Dissociation Energy
- Band Shape
- Excited State Analysis

End of Module Checkpoint

Module 3

All-Atom Molecular Dynamics

6 hours + Comp Time

Video: Introduction to Molecular Dynamics (MD)

Tutorials:

- Disordered System Building and MD Multistage Workflows
- Molecular Deposition
- Kinetic Monte Carlo Charge Mobility
- Molecular Dielectric Properties

End of Module Checkpoint

Module 4

Machine Learning

3 hours + Comp Time

Video: Introduction to Machine Learning (ML)

Tutorials:

- Machine Learning for Materials Science
- Optoelectronics Active Learning

End of Module Checkpoint

Module 5

Guided Case Study

3 hours + Comp Time

Tutorial: Modeling Intermolecular Interactions in the Emissive Layer

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: Evaluating Hole Transport Materials

Evaluated for Certification

Homogeneous Catalysis and Reactivity

Module 1

Introduction to Materials Modeling

2 hours

Video: Introduction to Materials Modeling & This Online Course

Video Tutorial: Introduction to Materials Science (MS) Maestro

Video: Modeling for Homogeneous Catalysis and Reactivity

Module 2

Molecular Quantum Mechanics

7 hours + Comp Time

Video: Introduction to Molecular Quantum Mechanics (mQM)

Tutorials:

- Functionals, Basis Sets and Geometry Optimizations
- R-Group Enumeration
- QM Multistage Workflows
- Rigid & Relaxed Coordinate Scans
- Energies of Reactions
- Organometallic Complexes

End of Module Checkpoint

Module 3

Molecular Quantum Mechanics

7 hours + Comp Time

Tutorials:

- Bond and Ligand Dissociation Energy
- Beta Elimination Reactions
- Locating Transition States: Part One
- Locating Transition States: Part Two
- Reaction Workflow for Polyethylene Insertion

End of Module Checkpoint

Module 4

Machine Learning

3 hours + Comp Time

Video: Introduction to Machine Learning (ML)

Tutorials:

- Machine Learning for Materials Science
- Machine Learning for Homogeneous Catalysis

End of Module Checkpoint

Module 5

Guided Case Study

2 hours + Comp Time

Tutorial: Fundamental Organometallic Reactivity

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: Predicting Regioselectivity of Hydroboration

Evaluated for Certification

Surface Chemistry

Module 1

Introduction to Materials Modeling

2 hours

Video: Introduction to Materials Modeling & This Online Course

Video Tutorial: Introduction to Materials Science (MS) Maestro

Video: Modeling for Surface Chemistry

Module 2

Molecular & Periodic Quantum Mechanics

6 hours + Comp Time

Video: Introduction to Quantum Mechanics (mQM & pQM)

Tutorials:

- Functionals, Basis Sets and Geometry Optimizations
- QM Multistage Workflows
- Energies of Reactions
- Building and Manipulating Crystals
- Properties of Bulk Crystals

End of Module Checkpoint

Module 3

Molecular & Periodic Quantum Mechanics

5 hours + Comp Time

Tutorials:

- Modeling Surfaces
- Activation Energies for Reactivity in Solids and on Surfaces
- R-Group Enumeration
- Organometallic Complexes
- Beta Elimination Reactions
- Bond and Ligand Dissociation

End of Module Checkpoint

Module 4

Machine Learning

3 hours + Comp Time

Video: Introduction to Machine Learning (ML)

Tutorials:

- Machine Learning for Materials Science
- Periodic Descriptors for Inorganic Solids

End of Module Checkpoint

Module 5

Guided Case Study

4 hours + Comp Time

Tutorials: Palladium Precursor Design

Heterogeneous Carbon Dioxide Reduction

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: Adsorption of Formaldehyde onto Palladium

Evaluated for Certification

Battery Materials

Module 1

Introduction to Materials Modeling

2 hours

Video: Introduction to Materials Modeling & This Online Course

Video Tutorial: Introduction to Materials Science (MS) Maestro

Video: Introduction to Modeling for Batteries

Module 2

Molecular & Periodic Quantum Mechanics

7 hours + Comp Time

Video: Introduction to Molecular and Periodic Quantum Mechanics (mQM & pQM)

Tutorials:

- Quantum Mechanical Workflows and Properties: Part 1
- Quantum Mechanical Workflows and Properties: Part 2
- Building Bulk Crystals and Calculating Properties
- Calculating Intercalation and Voltage Curves
- Lithium Ion Migration Barrier (NEB)

End of Module Checkpoint

Module 3

All-Atom Molecular Dynamics

6 hours + Comp Time

Video: Introduction to Molecular Dynamics (MD)

Tutorials:

- Disordered System Building and MD Multistage Workflows
- Building, Equilibrating and Analyzing Polymers
- Diffusion
- Polymer Electrolyte Analysis
- Liquid Electrolyte Properties: Part 1
- Liquid Electrolyte Properties: Part 2

End of Module Checkpoint

Module 4

Machine Learning

3 hours + Comp Time

Video: Introduction to Machine Learning (ML)

Tutorials:

- Machine Learning for Materials Science
- Machine Learning for Ionic Conductivity

End of Module Checkpoint

Module 5

Guided Case Study

3 hours + Comp Time

Tutorial: EC Decomposition on a Li (001) Surface

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: Modifying Battery Electrolyte Components

Evaluated for Certification

Pharmaceutical Formulations

Module 1

Introduction to Materials Modeling

2 hours

Video: Introduction to Materials Modeling & This Online Course

Video Tutorial: Introduction to Materials Science (MS) Maestro

Video: Modeling for Pharmaceutical Formulations

Module 2

All-Atom Molecular Dynamics

6 hours + Comp Time

Video: Introduction to Molecular Dynamics (MD)

Tutorials:

- Disordered System Building and MD Multistage Workflows
- Molecular Dynamics Simulations for API (active pharmaceutical ingredient) Miscibility
- Glass Transition Temperature for APIs
- Hygroscopicity
- Crystal Morphology

End of Module Checkpoint

Module 3

Coarse-Grained Simulation

5 hours + Comp Time

Video: Introduction to Coarse-Graining (CG)

Tutorials:

- Ibuprofen Cyclodextrin Inclusion Complexes with the Martini Coarse-Grained Force Field
- Ibuprofen Copovidone Drug Excipient Model with Dissipative Particle Dynamics (DPD)

End of Module Checkpoint

Module 4

Molecular & Periodic Quantum Mechanics

5 hours + Comp Time

Video: Introduction to Quantum Mechanics (mQM & pQM)

Tutorials:

- Functionals, Basis Sets and Geometry Optimizations
- QM Multistage Workflows
- Bond and Ligand Dissociation Energy
- pKa
- Building and Manipulating Crystals
- Properties of Bulk Molecular Crystals

End of Module Checkpoint

Module 5

Guided Case Study

2 hours + Comp Time

Tutorial: Nanoemulsions with Automated DPD Parameterization

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: API Property Prediction

Evaluated for Certification

Polymeric Materials

Module 1

Introduction to Materials Modeling

2 hours

Video: Introduction to Materials Modeling & This Online Course

Video Tutorial: Introduction to Materials Science (MS) Maestro

Video: Modeling for Polymeric Materials

Module 2

Molecular Dynamics

7 hours + Comp Time

Video: Introduction to Molecular Dynamics (MD)

Tutorials:

- Disordered System Building and MD Multistage Workflows
- Building, Equilibrating and Analyzing Polymers
- Building Polymer-Polymer Interfaces
- Crosslinking Polymers

End of Module Checkpoint

Module 3

Molecular Dynamics

6 hours + Comp Time

Tutorials:

- Polymer Property Prediction
- Penetrant Loading
- Diffusion
- Polymer Electrolyte Analysis
- Dielectric Properties

End of Module Checkpoint

Module 4

Machine Learning

3 hours + Comp Time

Video: Introduction to Machine Learning (ML)

Tutorials:

- Machine Learning for Materials Science
- Polymer Descriptors for Machine Learning

End of Module Checkpoint

Module 5

Guided Case Study

2 hours + Comp Time

Tutorial: Epoxy Formulations

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: Polymer-Mediated Graphene Dispersion

Evaluated for Certification

Consumer Packaged Goods

Module 1

Introduction to Materials Modeling

2 hours

Video: Introduction to Materials Modeling & This Online Course

Video Tutorial: Introduction to Materials Science (MS) Maestro

Video: Modeling for Consumer Packaged Goods

Module 2

Molecular Dynamics

7 hours + Comp Time

Video: Introduction to Molecular Dynamics (MD)

Tutorials:

- Disordered System Building and MD Multistage Workflows
- Building, Equilibrating and Analyzing Polymers
- Building a Carbohydrate Polymer
- Building Polymer-Polymer Interfaces
- Crosslinking Polymers

End of Module Checkpoint

Module 3

Molecular Dynamics & Coarse-Grained Simulation

6 hours + Comp Time

Tutorials:

- Cluster Analysis
- Surfactant Tilt and Electrostatic Potential
- Viscosity
- Starch Moisture Uptake and Plasticization

Video: Introduction to Coarse-Graining

Tutorials:

- Building a Coarse-Grained Surfactant Model

End of Module Checkpoint

Module 4

Machine Learning

3 hours + Comp Time

Video: Introduction to Machine Learning (ML)

Tutorials:

- Machine Learning for Materials Science
- Polymer Descriptors for Machine Learning
- Machine Learning for Sweetness

End of Module Checkpoint

Module 5

Guided Case Study

2 hours + Comp Time

Tutorial: Coarse-Grained Modeling of SLES

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: Self-Aggregation of DDM and DPC Molecules

Evaluated for Certification

Teaching with Schrödinger

Teaching with Schrödinger

Schrödinger's suite of software is now easily accessible to students and educators.

About

- Build, calculate, and analyze structures for teaching purposes using web-based Maestro (Small Molecule Drug Discovery, Biologics Discovery, & Materials Science)
- No need for students or instructors to download software—access is through a virtual desktop environment via a web browser

Resources

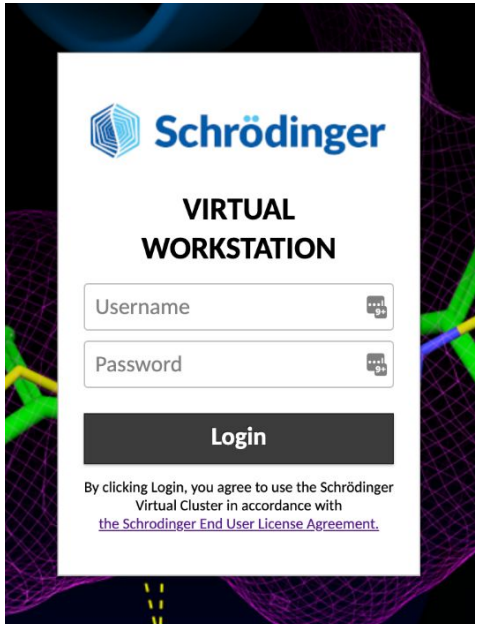
- Educational materials in a variety of chemistry and biology subjects at the undergraduate and high school levels (i.e. General Chemistry, Organic Chemistry, Medicinal Chemistry, etc.)
- Readily available lab assignments, lesson plans, and worksheets with computational exercises for students and instructors to use

Support

- No computational experience? No problem! We will provide support for students and instructors on how to use the Maestro interface and perform basic functions
- Included with a purchase are in-class demos with a Schrödinger Education Team member

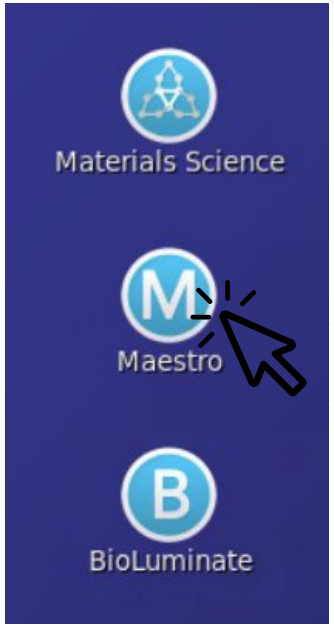
Teaching with Schrödinger Program: How Does It Work?

Login through a Web Browser



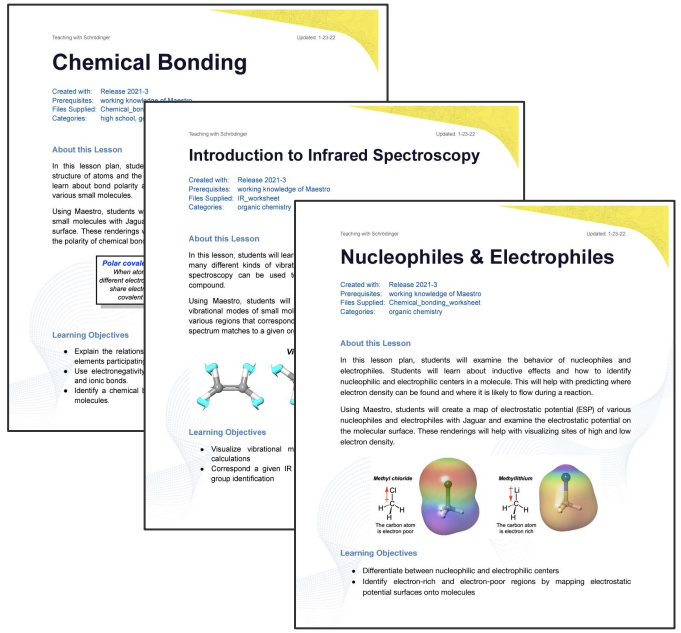
- Instructors and students use their user credentials to login using a web browser

Open Web-Based Maestro



- Access industry-grade, web-based Maestro directly on the virtual workstation

Perform Calculations



- Import, build, calculate, visualize, and analyze molecular structures

Teaching with Schrödinger Pre-Configured Lessons

General Chemistry

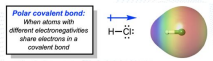
Chemical Bonding

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: Chemical_bonding_worksheet
Categories: high school, general chemistry 1

About this Lesson

In this lesson plan, students will examine the relationship between the electronic structure of atoms and the ionic and covalent chemical bonds they form. Students will learn about bond polarity and electronegativity by looking at electron distributions of various small molecules.

Using Maestro, students will create a map of electrostatic potential (ESP) of various small molecules with Jaguar and examine the electrostatic potential on the molecular surface. These renderings will help with visualizing electronegativity trends and gauging the polarity of chemical bonds.



Learning Objectives

- Explain the relationship between the type of bonding and the properties of the elements participating in the bond.
- Use electronegativity differences to identify nonpolar covalent, polar covalent, and ionic bonds.
- Identify a chemical bond type by mapping electrostatic potential surfaces onto molecules.

VSEPR Theory

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: VSEPR_theory_worksheet, glycine.mae
Categories: high school, general chemistry 1

About this Lesson

In this lesson plan, students will examine the three-dimensional shapes and sizes of molecules through the VSEPR model by analyzing their bond angles and bond lengths. Starting with Lewis structures, students will identify the regions of electron density around a central atom and analyze the best fit molecular geometry.

Using Maestro, students will build and optimize molecular geometries with Jaguar and measure bond distances and angles to predict geometric arrangements. These calculations will help with visualizing how certain geometries better minimize electron repulsions than others.

Learning Objectives

- Use Lewis structures and the valence shell electron-pair repulsion (VSEPR) model to create and predict shapes of molecules
- Perform quantum mechanical calculations to optimize molecular geometries and measure bond distances and angles of various small molecules

Organic Chemistry

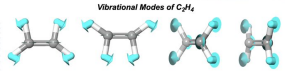
Introduction to Infrared Spectroscopy

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: IR_worksheet
Categories: organic chemistry

About this Lesson

In this lesson, students will learn the fundamentals of infrared (IR) spectroscopy and the many different kinds of vibrational excitation, including stretching and bending. IR spectroscopy can be used to identify which functional groups are present in a compound.

Using Maestro, students will perform frequency calculations and visualize various vibrational modes of small molecules. Students will then generate IR spectra, identify various regions that correspond to particular functional groups, and determine which IR spectrum matches to a given organic compound.



Learning Objectives

- Visualize vibrational modes of small molecules by performing frequency calculations
- Correspond a given IR spectrum to an organic compound through functional group identification

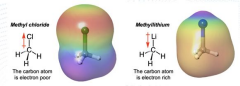
Nucleophiles & Electrophiles

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: Chemical_bonding_worksheet
Categories: organic chemistry

About this Lesson

In this lesson plan, students will examine the behavior of nucleophiles and electrophiles. Students will learn about inductive effects and how to identify nucleophilic and electrophilic centers in a molecule. This will help with predicting where electron density can be found and where it is likely to flow during a reaction.

Using Maestro, students will create a map of electrostatic potential (ESP) of various nucleophiles and electrophiles with Jaguar and examine the electrostatic potential on the molecular surface. These renderings will help with visualizing sites of high and low electron density.



Learning Objectives

- Differentiate between nucleophilic and electrophilic centers
- Identify electron-rich and electron-poor regions by mapping electrostatic potential surfaces onto molecules

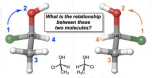
Stereoisomers

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: Stereoisomers_worksheet
Categories: organic chemistry

About this Lesson

In this lesson plan, students will explore compounds called stereoisomers that differ from each other only in the three-dimensional, spatial arrangement of their atoms, but not in the connectivity of their atoms. The connection between stereoisomerism and drug action will also be discussed.

Using Maestro, students will use the 2D Sketcher and 3D Builder tools to learn how to draw different kinds of stereoisomers. Energy minimizations and geometry optimization calculations will be performed using Jaguar. The tile function will be used to compare stereoisomeric relationships between pairs of molecules to determine if they are enantiomers or diastereomers.



Learning Objectives

- Designate configuration of a stereocenter using the Cahn-Ingold-Prelog (CIP) system
- Determine the stereochemical relationship between a pair of molecules

Substitution Nucleophilic (S_N2) Reactions

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: SN2_reactions_worksheet
Categories: organic chemistry

About this Lesson

In this lesson plan, students will examine bimolecular substitution nucleophilic (S_N2) reactions. Transition state theory will be introduced to analyze the concerted mechanism of how a nucleophile attacks an electrophile to form a given product. Reaction energy diagrams will be investigated to determine whether a reaction is exergonic or endergonic.

Using Maestro, students will use Jaguar's AutoTS panel to perform geometry optimization calculations of the reactants and products of an S_N2 reaction, determine which bonds are breaking and forming, establish correspondence between atoms in the reactants and the products, and generate a transition state structure. Then, they will render a potential energy surface diagram to show the activation energy barrier.

Learning Objectives

- Identify transition state structures of S_N2 reaction mechanisms
- Plot reaction energy diagrams with activation energy barriers to determine their chemical reactivity characteristics (i.e. endergonic, exergonic, etc.)

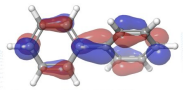
Advanced Orgo

HOMO-LUMO Energy Gap

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: HOMO_LUMO_worksheet
Categories: general chemistry, organic chemistry

About this Lesson

Using Maestro, students will use the 2D Sketcher to learn how to draw small molecules. Energy minimizations and geometry optimization calculations will be performed using Jaguar. Molecular orbital surfaces of the HOMO and LUMO will also be calculated and visualized. HOMO-LUMO energy gaps can be found in the project table.



Learning Objectives

- Build a molecule using the 2D sketcher
- Run a Jaguar optimization calculation to generate the molecular orbital surfaces
- Visualize the HOMO and LUMO of a molecule
- Calculate the HOMO–LUMO energy gap using results in the Project Table

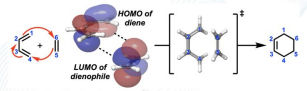
Diels-Alder Reactions

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: Diels_Alder_worksheet
Categories: organic chemistry

About this Lesson

In this lesson plan, students will examine the relationship between a diene and a dienophile in a Diels-Alder reaction. Transition state theory will be introduced to analyze the concerted mechanism of a [4+2] cycloaddition. Reaction energy diagrams will be investigated to determine whether a reaction is exergonic or endergonic.

Using Maestro, students will use Jaguar's AutoTS panel to calculate the energetics of the reactants, product, and transition state. Students will also calculate the HOMO and LUMO of reactants to help with visualizing π molecular orbital overlap.



Learning Objectives

- Identify transition state structures of Diels-Alder reaction mechanisms
- Plot reaction energy diagrams with activation energy barriers to determine their chemical reactivity characteristics (i.e. endergonic, exergonic, etc.)
- Generate molecular orbitals of the diene and dienophile to analyze favorable orbital overlap for product formation

Biochemistry

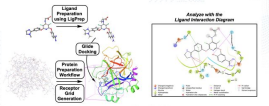
Protein Ligand Docking

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: Protein_ligand_docking_worksheet
Categories: biochemistry, medicinal chemistry

About this Lesson

Determining the binding mode of an active molecule to a given protein target is important in the drug discovery pipeline. This lesson will focus on reproducing an experimentally observed binding mode through docking.

Using Maestro, students will learn how to import a .pdb file of a crystal structure, prepare a protein and ligand, as well as dock a ligand into a protein receptor using Schrödinger's Glide. They will also analyze protein-ligand interactions from a Ligand Interaction Diagram.



Learning Objectives

- Prepare ligand and protein structures in Maestro
- Learn the steps of a molecular docking workflow using Schrödinger's Glide
- Analyze integral protein-ligand interactions within an active site using the Ligand Interaction Diagram

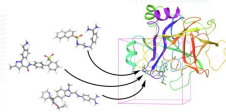
Structure-Based Virtual Screening

Created with: Release 2021-3
Prerequisites: working knowledge of Maestro
Files Supplied: SBVS_worksheet
Categories: biochemistry, medicinal chemistry

About this Lesson

This lesson will focus on an important early stage of drug discovery in which protein structures and molecular modeling are utilized to identify molecules that can be further developed into drugs.

Using Maestro, students will learn how to perform a virtual screen for potential inhibitors of FXa using the ligand docking application Glide. Students will learn how to generate a protein receptor grid, dock a set of ligands into the receptor grid, and analyze the docking results. Students can then sketch their own inhibitor designs and evaluate their value.

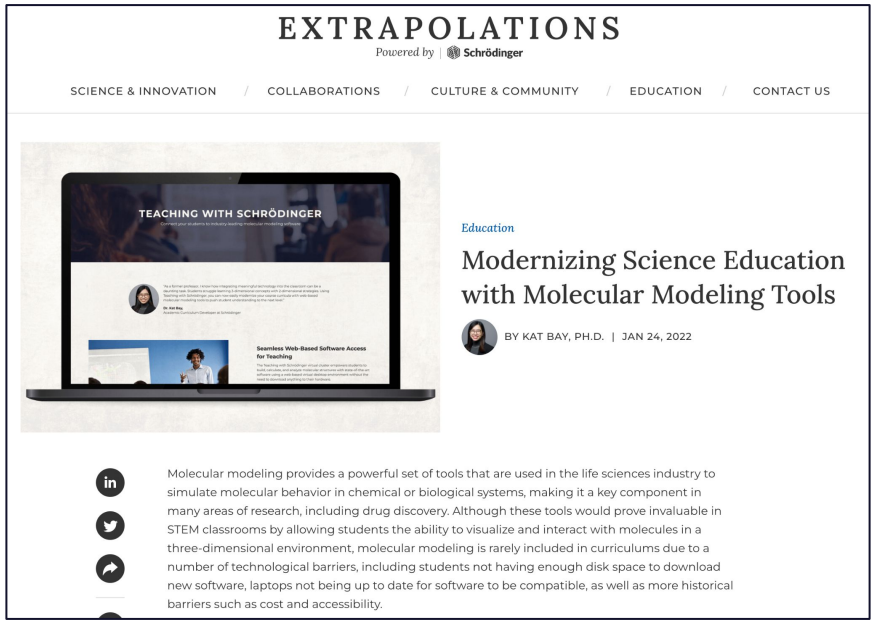


Learning Objectives

- Learn the steps of a molecular docking workflow using Schrödinger's Glide
- Perform a structure-based virtual screen of a small set of ligands
- Design your own inhibitor for FXa and determine its docking score

Industry-Leading Molecular Modeling in the Classroom

Modernizing Science Education with Molecular Modeling Tools Blog Post



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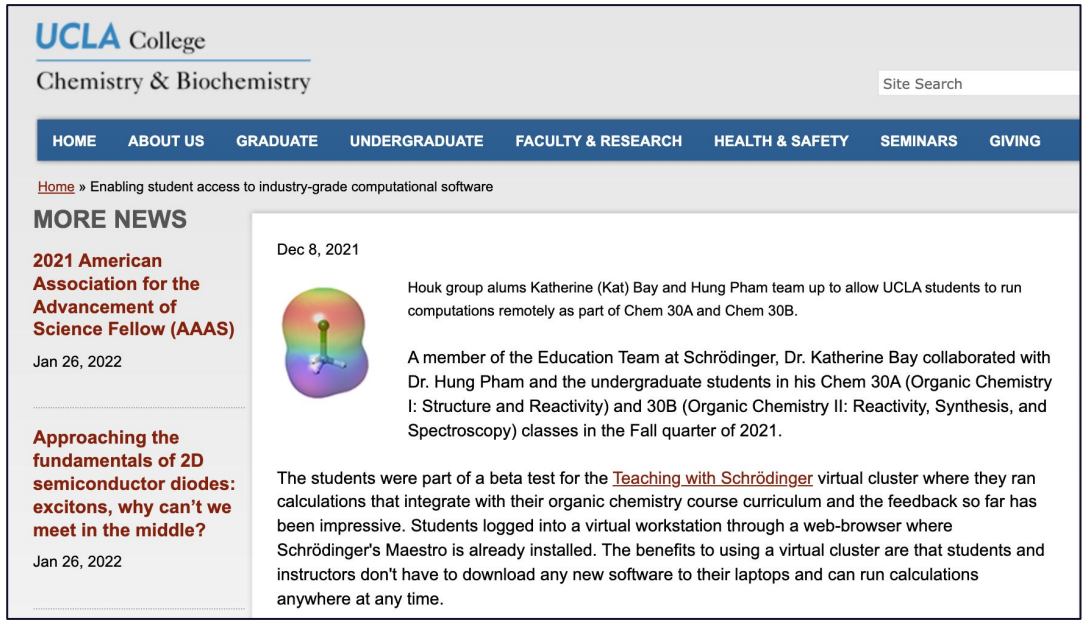
See how UCLA students use Maestro in their courses



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*"**There is a huge boom now in companies looking for computational chemists, particularly for drug discovery.** The challenge is that many people don't necessarily get exposed to it in school, and I think we are missing out on students who would really like this kind of experience."*

- Prof. Severin Schneebeli
Associate Professor of Chemistry at University of Vermont

*"**Teaching with Schrödinger has undoubtedly prepared me for my future studies.** Providing students with industry-standard software expertise early on will make us better candidates for the real world."*

- Samantha Lee
Bioinformatics Undergraduate Student at New York City College of Technology

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