Schrödinger

Innovating with Schrödinger in the Batteries Industry

Schrödinger's commitment to innovation and support

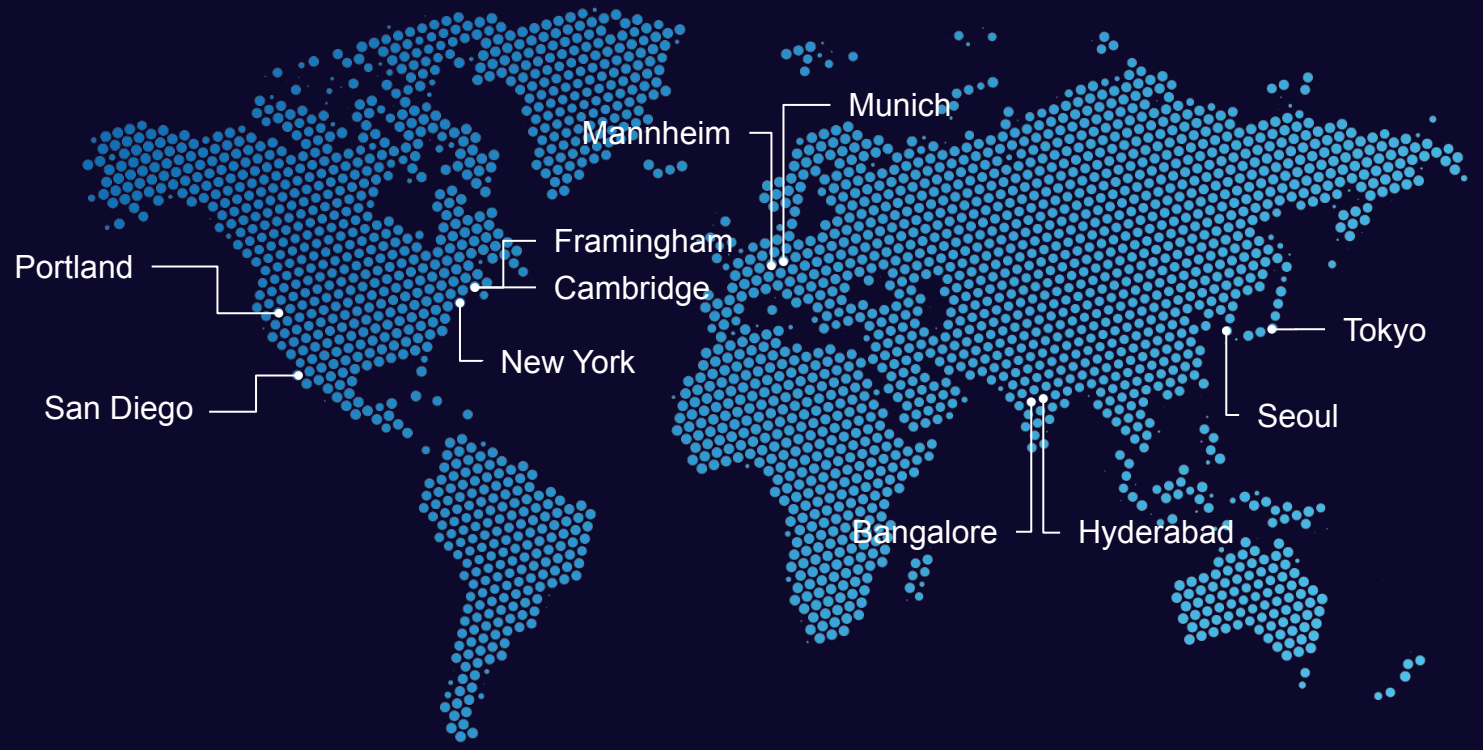
30+ years of innovation in molecular modeling

> 800 employees worldwide; > 40% Ph.D.

More than 50% of the company dedicated to R&D

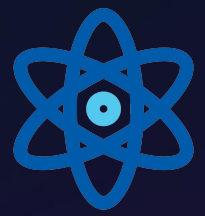
Large scientific support & education teams

Quarterly software releases with improvements



Computational methods

Schrödinger's digital chemistry platform leverages two classes of computational methods: physics-based modeling (e.g. quantum mechanics and molecular dynamics) and machine learning (e.g. cheminformatics, ML/AI)



Physics-based modeling

Machine learning

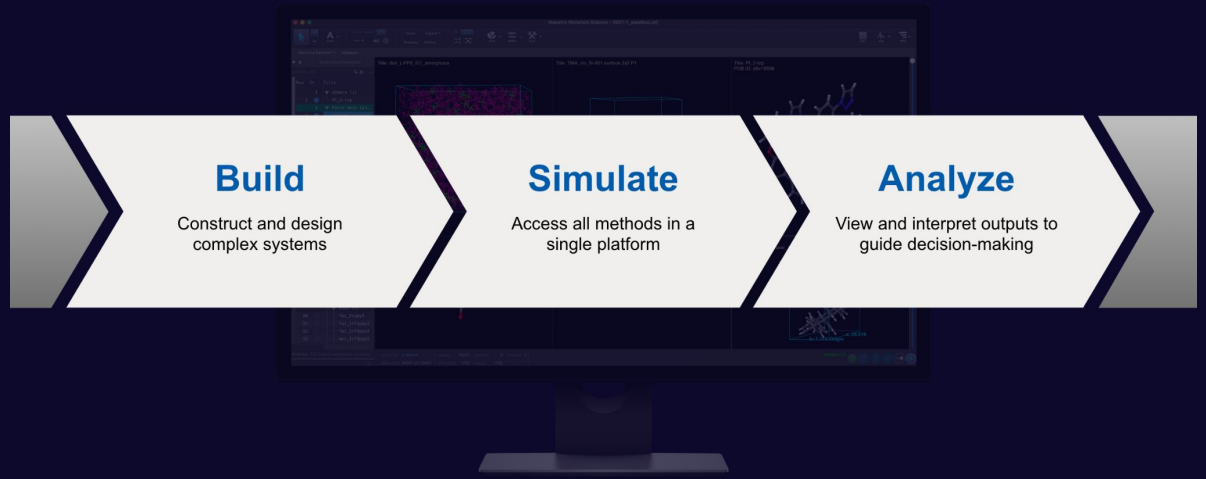
These synergistic approaches enable:

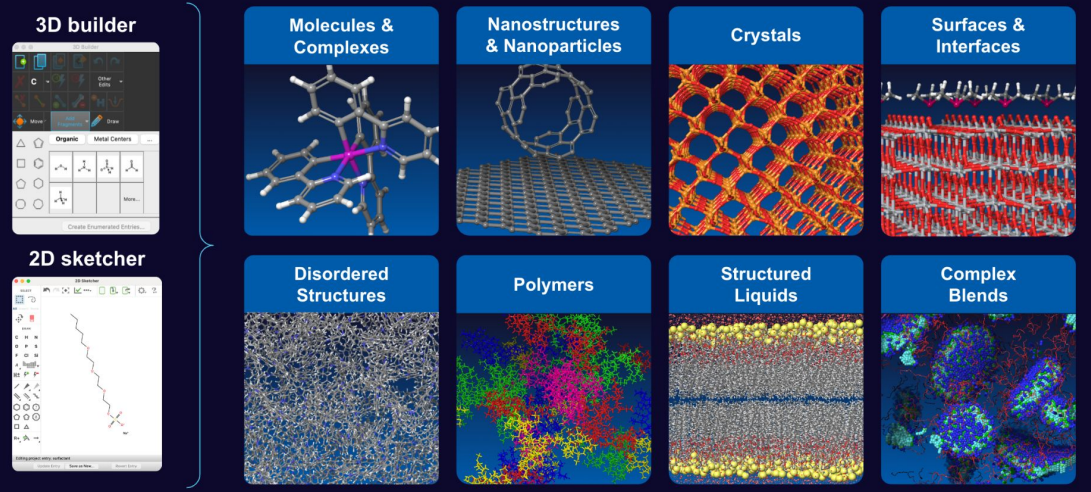
- Virtual screening of chemical libraries and de novo design of new materials
- In silico property prediction across a wide range of materials
- Increased understanding of materials behavior (e.g. root cause analysis, failure mechanism, recyclability)

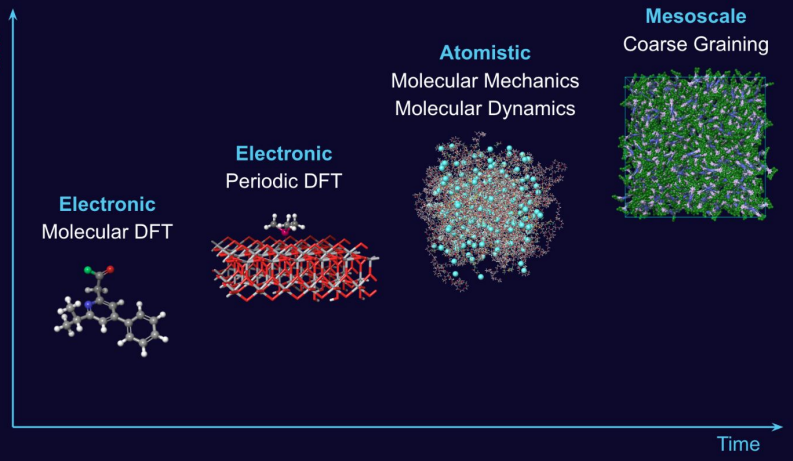
reducing **cost** and **risk** in materials innovation

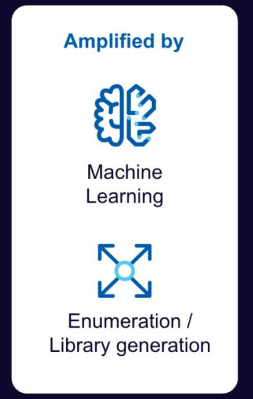
Physics-based modeling

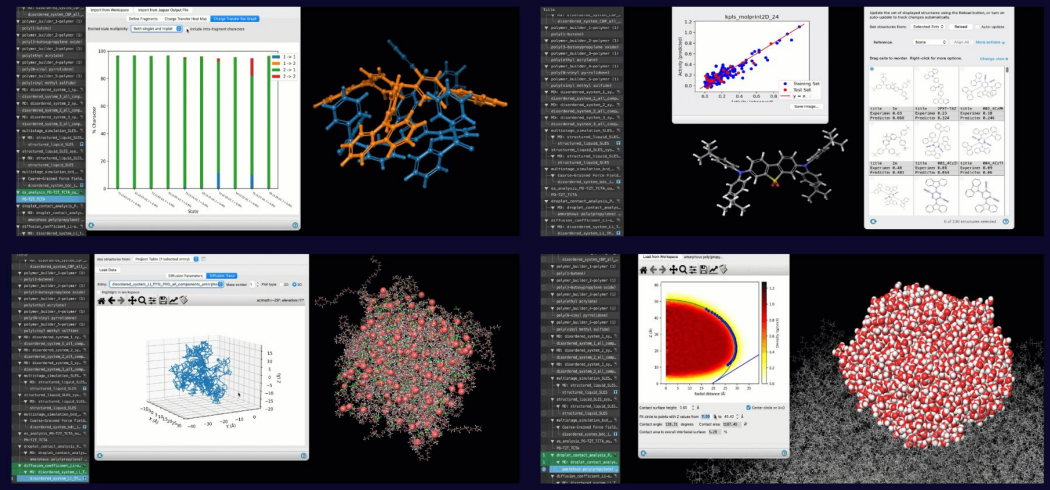
Fast and accurate engines enable high-throughput and multi-scale physics-based modeling approaches





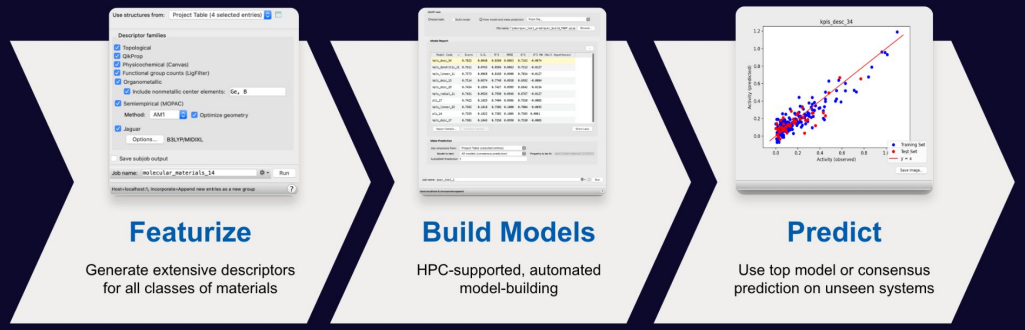






Machine learning

Generate descriptors and leverage automated model-building solutions for cheminformatics machine learning



Featurize

Generate extensive descriptors for all classes of materials

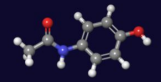
Build Models

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

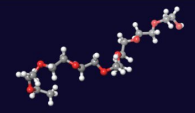


Small molecules

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

Physics-based descriptors:

- Quantum mechanics
- Auto Reaction Workflow

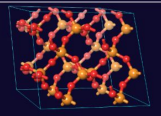


Polymers

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

Physics-based descriptors:

- Molecular dynamics
- Quantum mechanics

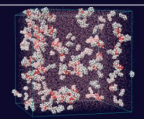


Periodic inorganic solids

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

Physics-based descriptors:

- Periodic quantum mechanics

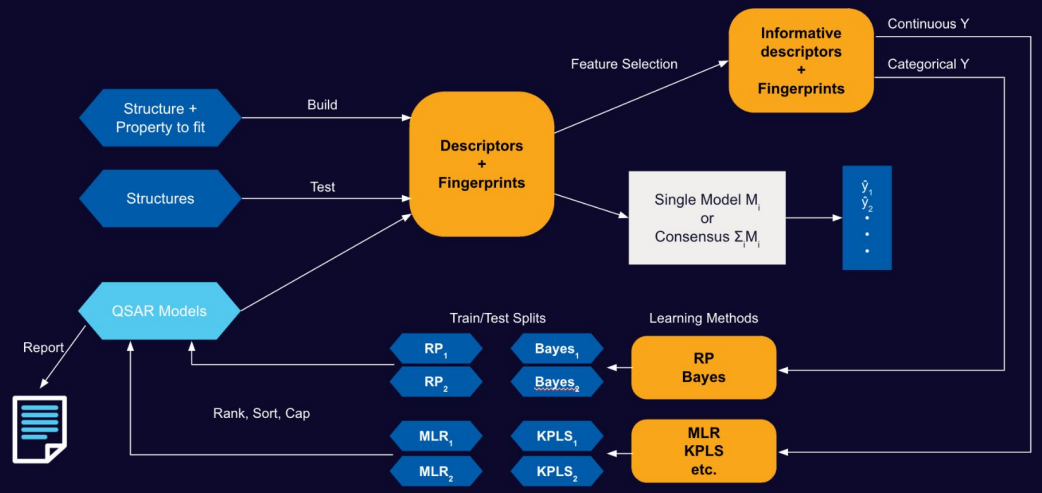


Formulations and mixtures

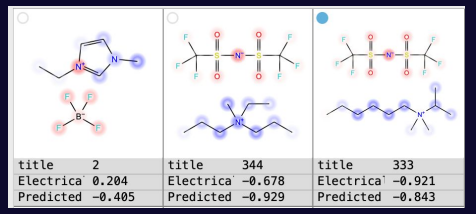
- Composition
- Chemistry of the components
- Experimental/processing conditions

Physics-based descriptors:

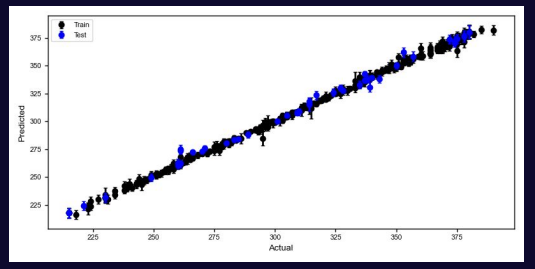
- Molecular dynamics

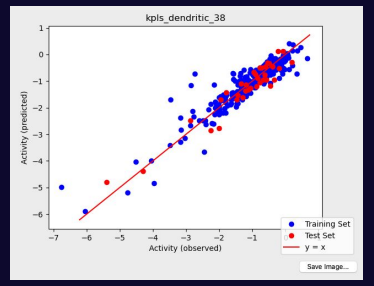


Model Code	Score	S.D.	R^2	RMSE	Q^2	Q^2 MW (Null
kpls_dendritic_38	0.8590	0.3468	0.8584	0.3451	0.9036	-0.0071
kpls_linear_38	0.8319	0.3664	0.8415	0.3770	0.8849	-0.0071
kpls_linear_40	0.8277	0.4017	0.8216	0.3384	0.8400	0.0146
kpls_dendritic_40	0.8159	0.4099	0.8142	0.3912	0.7862	0.0146
kpls_linear_23	0.8039	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

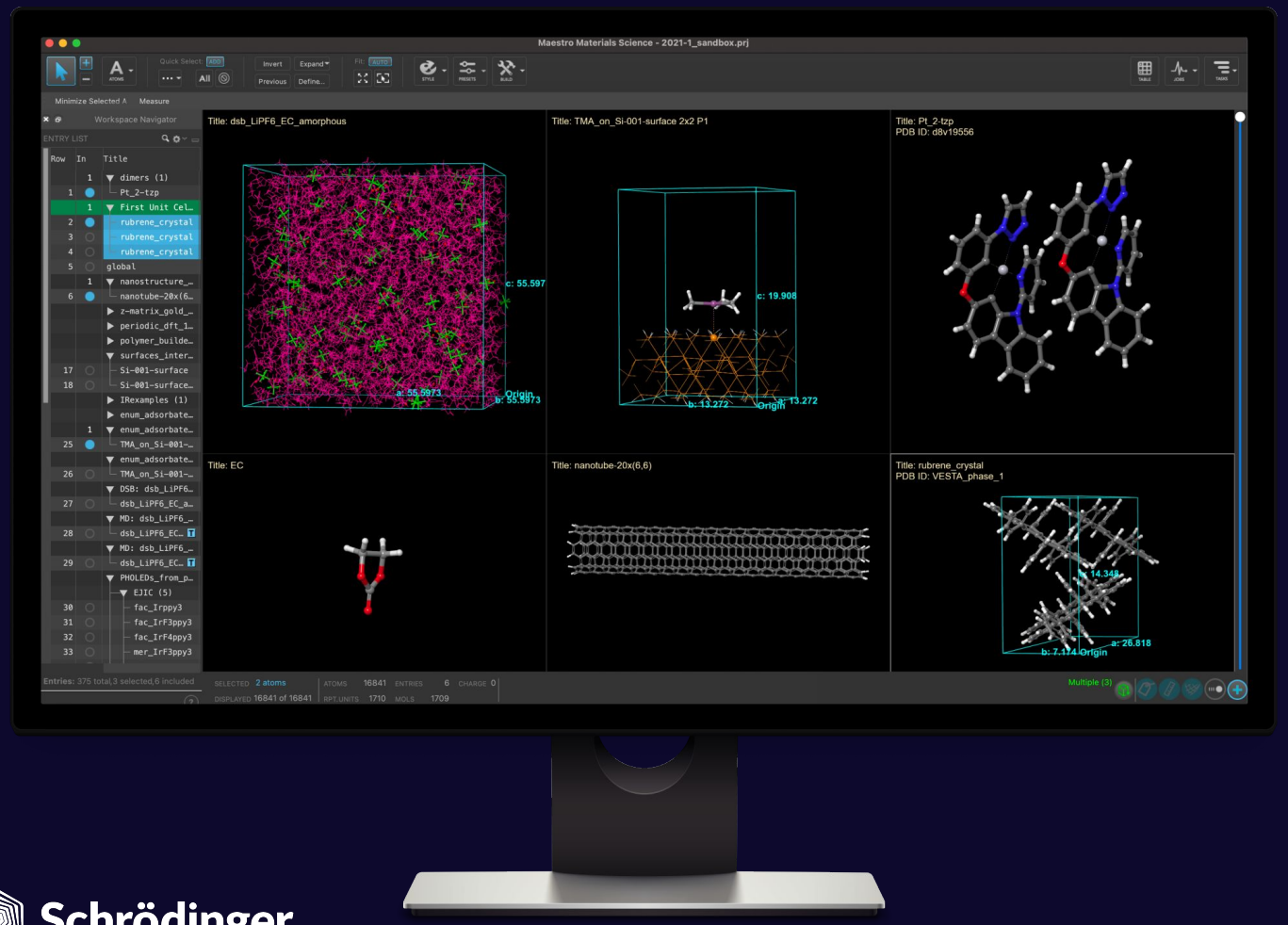




User-friendly GUI and comprehensive API

Everything that the Schrödinger platform offers is centered around a single, user-friendly graphical user interface, MS Maestro. Alternatively, for expert modelers, a comprehensive Python API enables programmatic interaction

MS Maestro



Python API

```
➜  ~ 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)
➜  ~
```

Jaguar

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

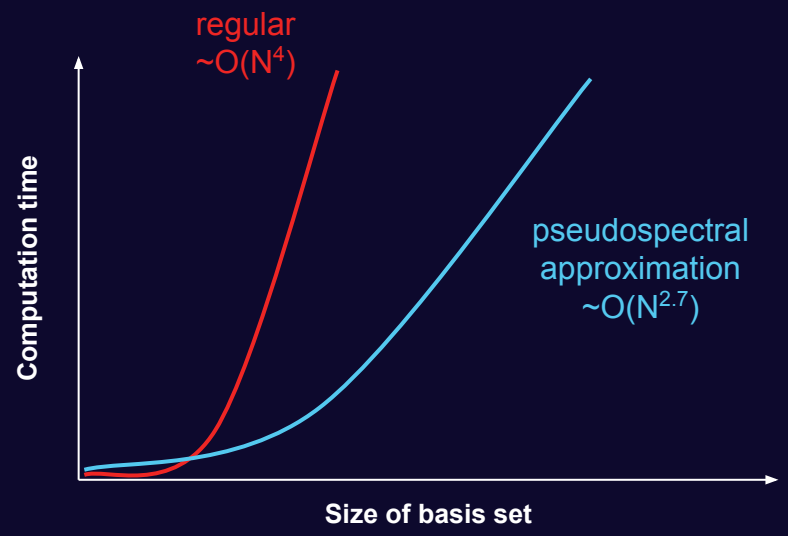
Key capabilities:

- 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

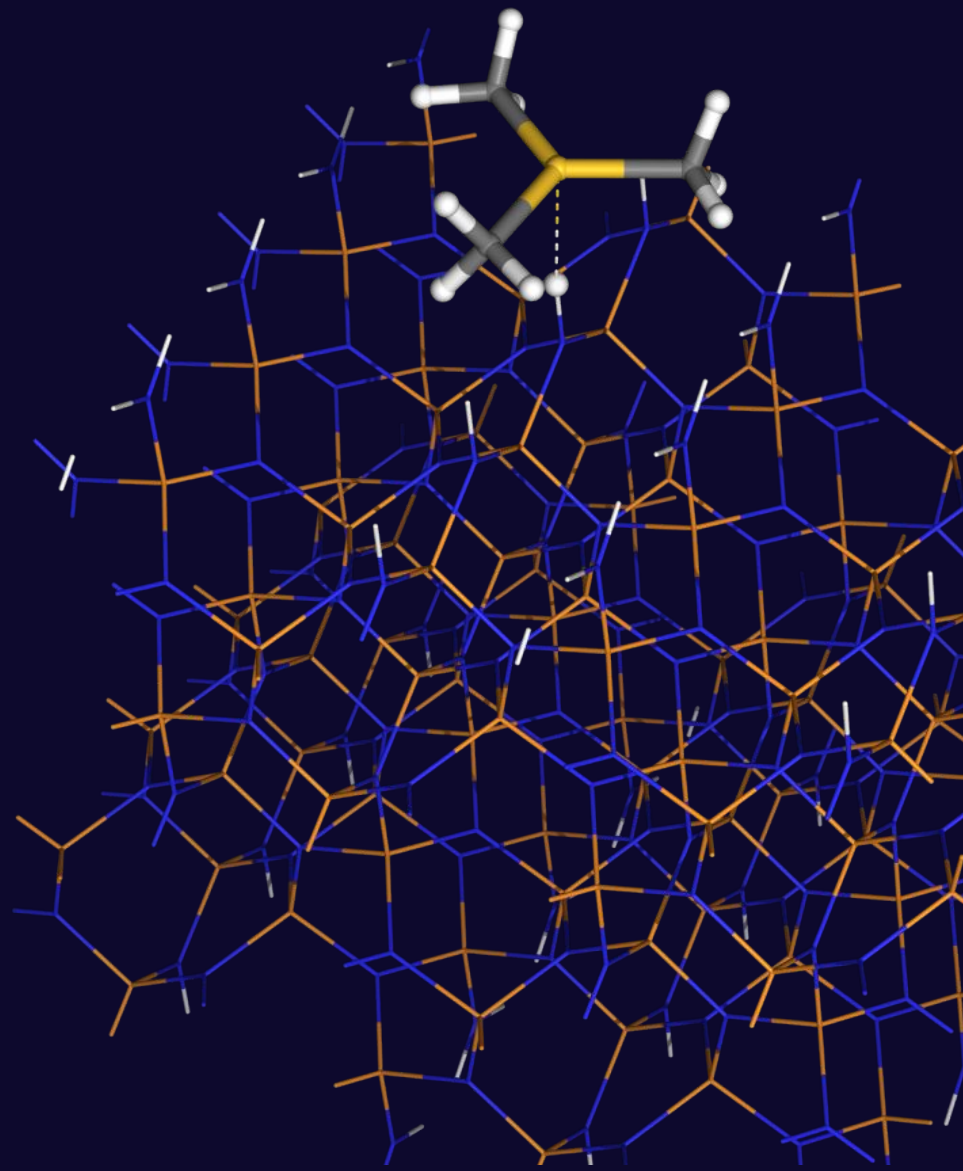


Schrödinger

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

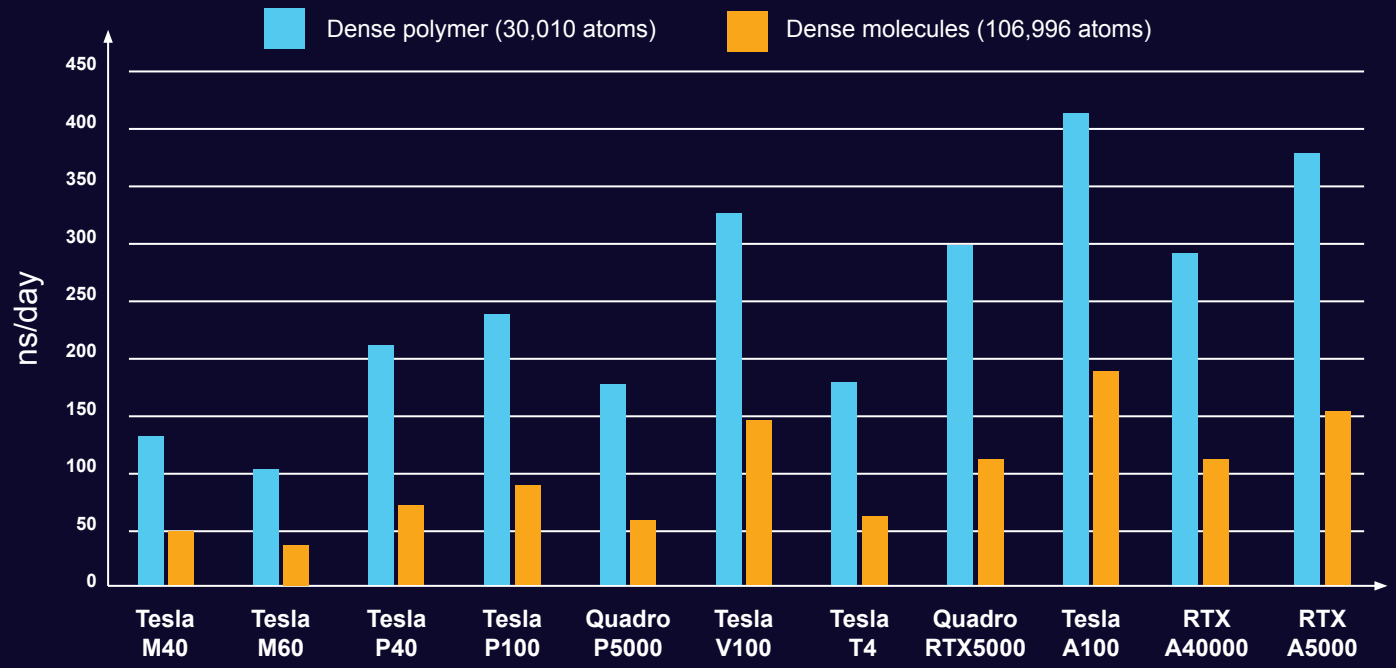
High-performance molecular dynamics (MD) engine providing high scalability, throughput, and scientific accuracy

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



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

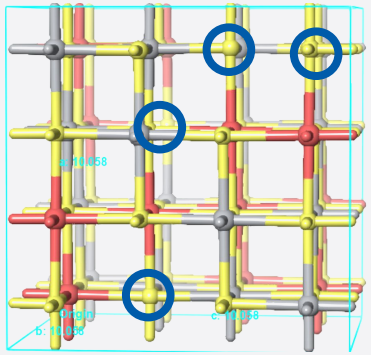
- Degradation
  - Bond dissociation energies
  - Prediction of decomposition products
- Reaction mechanism elucidation (molecules)
  - Energy landscape for reactants, intermediates, and products
  - Automated transition state search

Solid Electrolyte Interphase

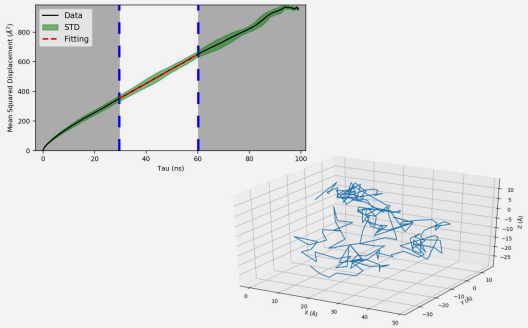
- Solid-electrolyte interphase simulator for constructing SEI models
  - Reaction-template-based molecular dynamics simulation with multiple reaction components
- Ab initio MD (AIMD) for the study of early stage SEI formation mechanisms
- Reaction mechanism elucidation (surfaces)
  - Energy landscape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

Energy capture and storage: select capabilities

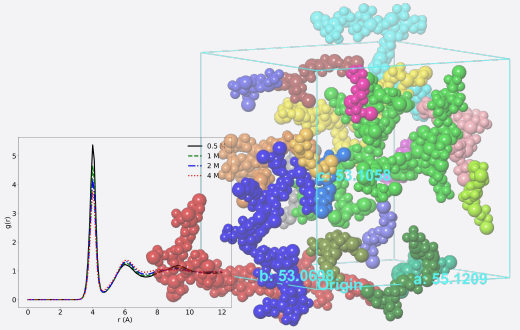
Electrode properties



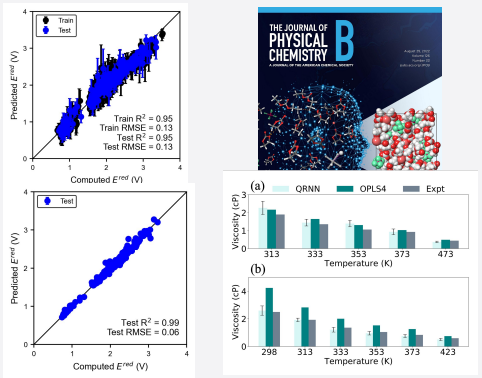
Transport properties: diffusion and viscosity



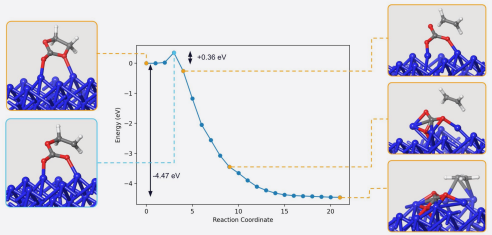
Electrolyte structure analysis



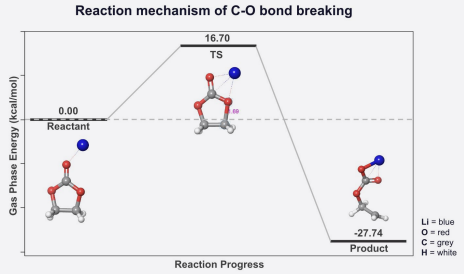
ML models and ML-FF



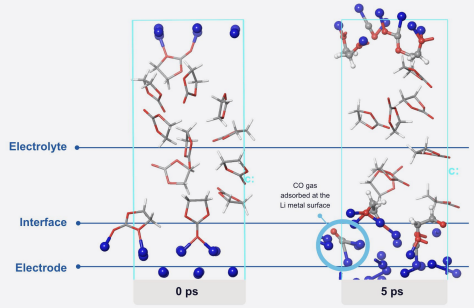
Surface reactivity



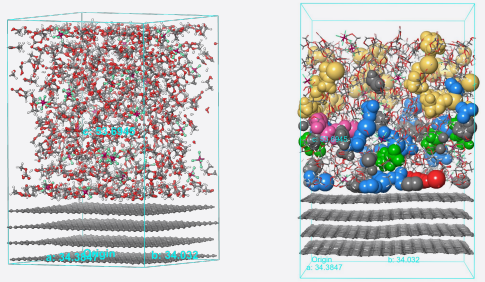
Small molecule reactivity



Electrolyte degradation

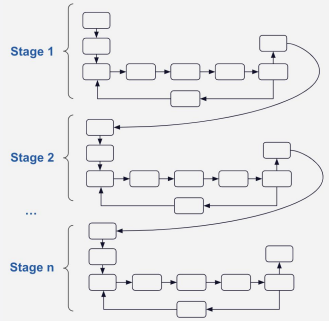


Solid electrolyte interphase morphology

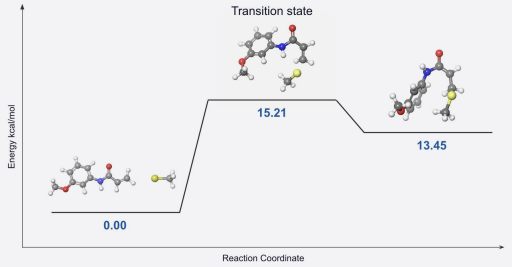


Catalysis and reactivity: select capabilities

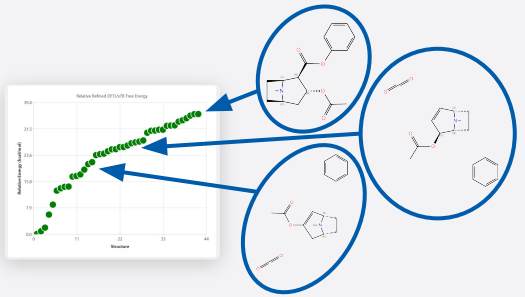
Multistage quantum mechanical solutions



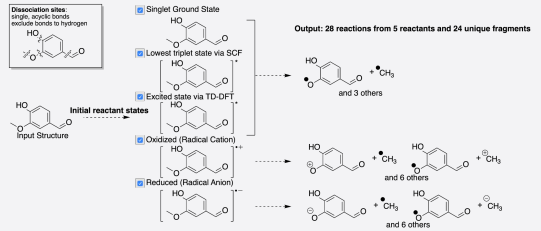
Automated transition state searching



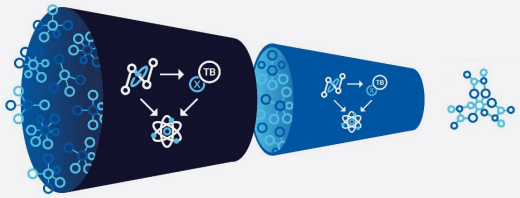
Degradation products prediction



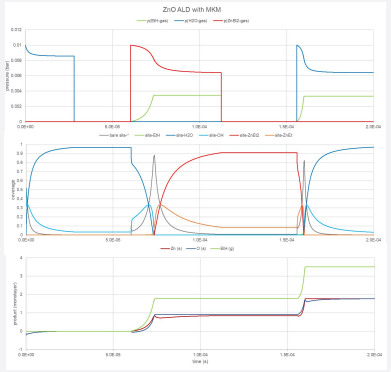
Bond dissociation energies



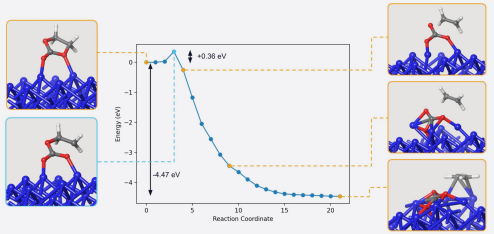
Molecular catalyst design



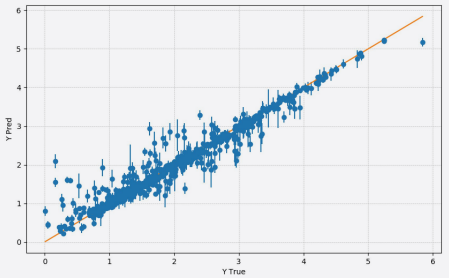
Microkinetic modeling



Surface reactivity

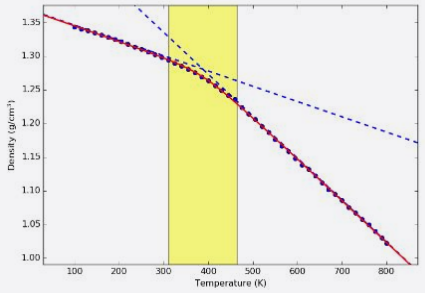


Cheminformatics for catalyst design

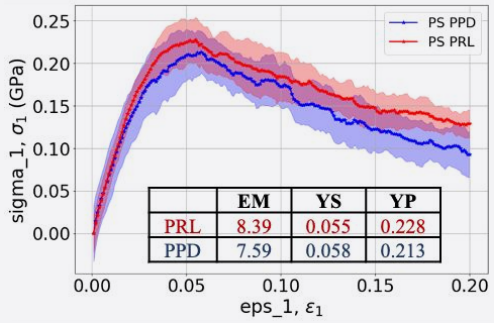


Polymeric materials: select capabilities

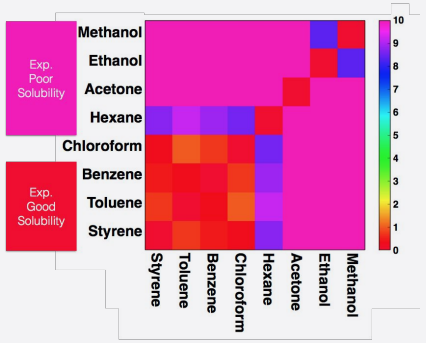
Glass transition temperature



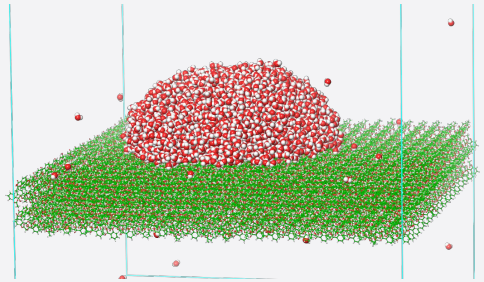
Mechanical response



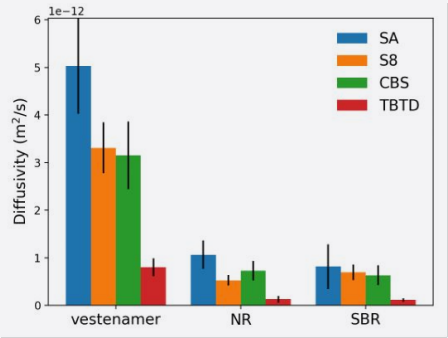
Miscibility and solubility



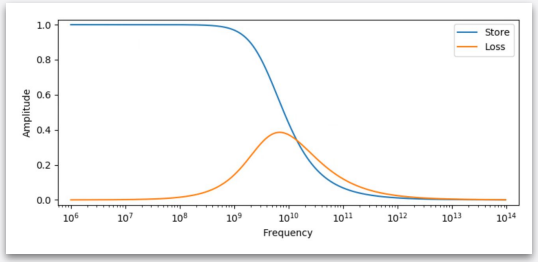
Contact angle



Diffusivity

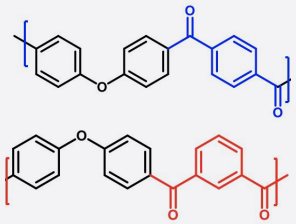


Dielectric properties



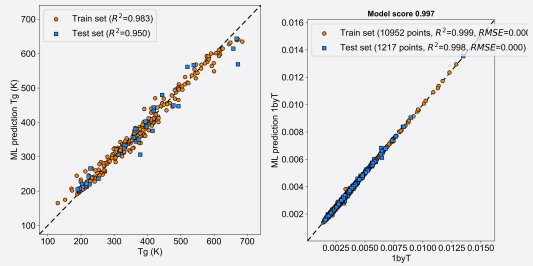
Bond dissociation energy

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



How to work with Schrödinger

Software License

Leverage molecular simulations in-house with extensive Schrödinger support

Contract Research & Development

Leverage Schrödinger scientific and engineering expertise to solve your research challenges and enable your workforce

How to work with Schrödinger

Software License

Leverage molecular simulations in-house with extensive Schrödinger support

Trust our extensive experience onboarding commercial customers:

- Dedicated science and technology support
- Professional online training courses, tutorials, and documentation
- Easy-to-use graphical interface with automated workflows (no coding required)
- No hardware? We can configure cloud resources for you

How to work with Schrödinger

Contract Research & Development

Leverage Schrödinger scientific and engineering expertise to solve your research challenges and enable your workforce

Trust our extensive experience executing research projects:

- Identify your important research questions to be addressed with simulation
- You retain the intellectual property
- No software or hardware needed
- Knowledge transfer and training available during and after the project

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
- Bond and Ligand Dissociation Energy
- Nanoreactor
- 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
- Solid Electrolyte Interphase Builder

End of Module Checkpoint

Module 4

Machine Learning

3 hours + Comp Time

Video: Introduction to Machine Learning (ML)

Tutorials:

- Machine Learning Property Prediction
- Machine Learning for Materials Science
- Machine Learning for Ionic Conductivity
- Molecular Dynamics Descriptors for Machine Learning
- Machine Learning for Formulations

End of Module Checkpoint

Module 5

Guided Case Study

3 hours + Comp Time

Case Studies: EC Decomposition on a Li (001) Surface

Ab initio Molecular Dynamics Simulations of Li-ion Diffusion in Solid-State Electrolytes

Module 6

Independent Case Study

4 hours + Comp Time

Assignment: Modifying Battery Electrolyte Components

Evaluated for Certification

Key Schrödinger advantages

	Open Source / Freeware	Other Commercial Software	**Schrödinger**
Usability	✓	✓ ✓	✓ ✓ ✓
Automated Solutions	✓	✓ ✓	✓ ✓ ✓
Speed and Accuracy	✓	✓ ✓	✓ ✓ ✓
Support	x	✓	✓ ✓ ✓
Training	x	x	✓ ✓ ✓
Contract Research	x	✓	✓ ✓ ✓

Read more about:

- Our Science
- Our People
- Our Training and Support
- Our Contract Research

All methods in the same interface, performed via GUI or command-line interface (Python API)

Automated solutions spanning multi-physics (e.g. QM, MD, ML) reflecting industry best practices

Extensively validated, fast and scalable engines (e.g. Jaguar, Desmond, OPLS force field)

Rapid, consultative support via email, phone, or hands-on with expert application scientists

70+ tutorials, complete documentation, and 7 industry-specific online certification courses

10+ year history of delivering modeling services projects across a variety of industries where deliverables are treated as customer IP

Thank you!

Contact:
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