Schrödinger

Modeling and Simulation for the Petrochemical Industry

2025

Commitment to innovation, software, and support

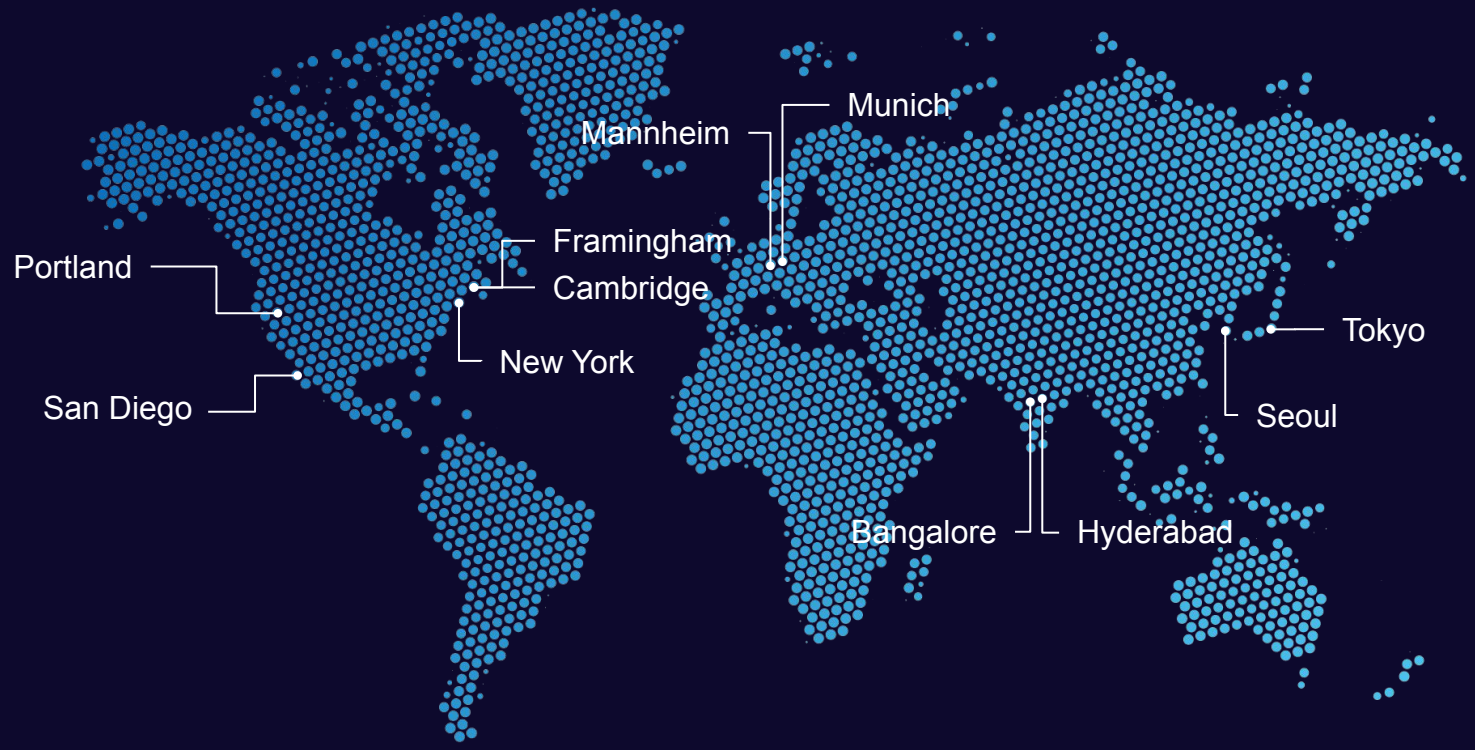
30+ years of innovation in molecular modeling

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

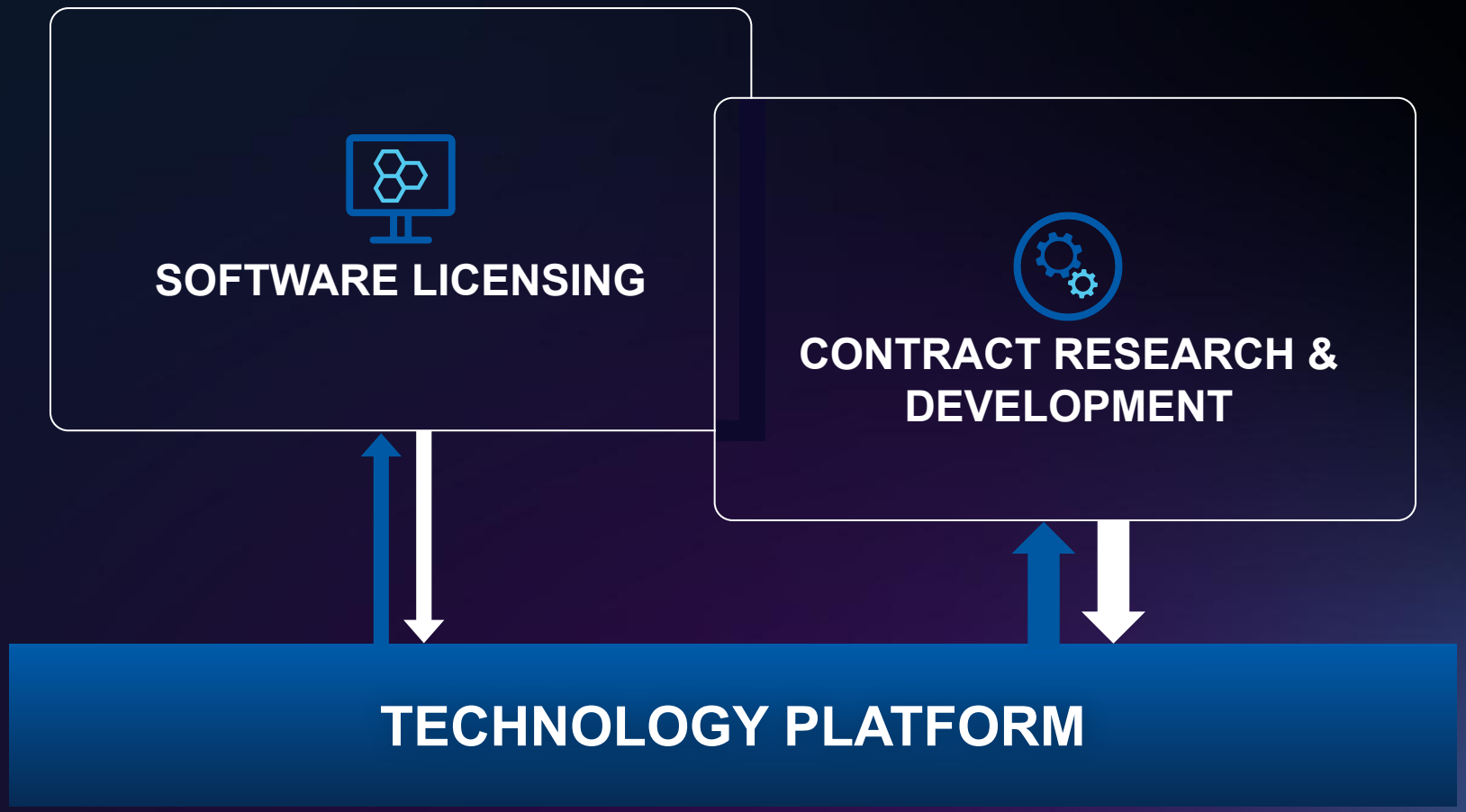
More than 50% of the company dedicated to R&D

Large scientific support & education teams

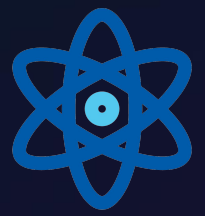
Quarterly software releases with improvements



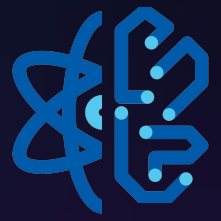
Engagement models



Synergy between physics-based modeling and machine learning



Physics-based modeling



Physics & Machine Learning

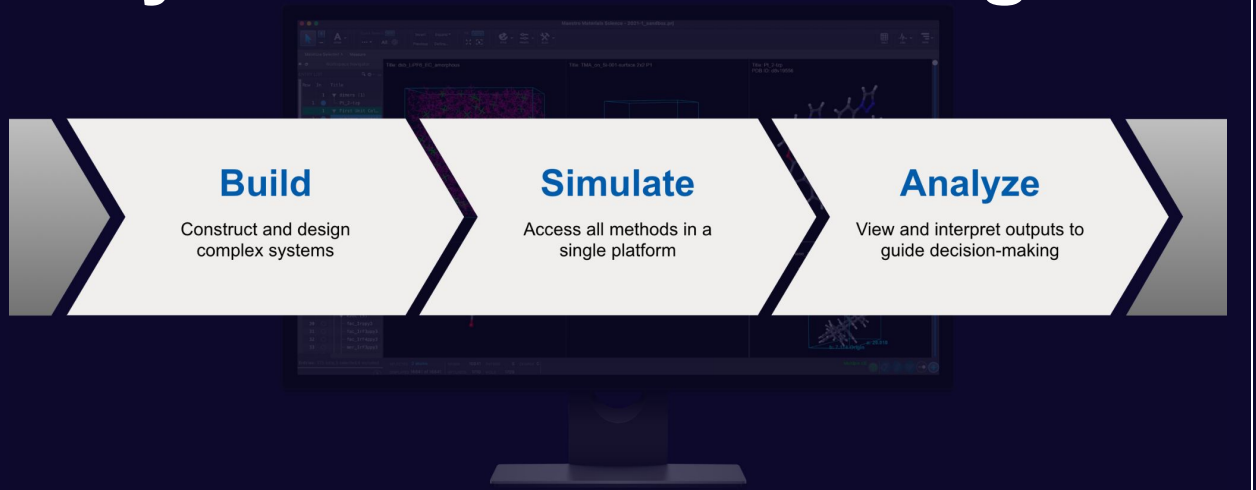
Incorporate physics-based information about materials into practical ML models.

Build targeted ML models to expand the impact of physics-based simulations.

Parameterize traditional physics-based approaches with ML.

Machine learning

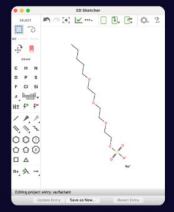
Physics-based modeling

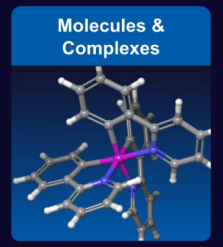


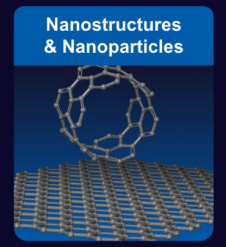
Build
Construct and design complex systems

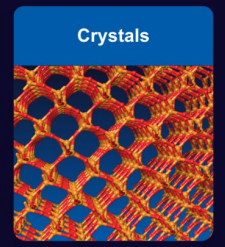
Simulate
Access all methods in a single platform

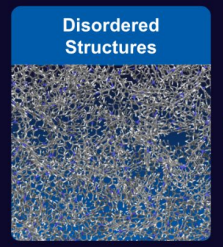
Analyze
View and interpret outputs to guide decision-making

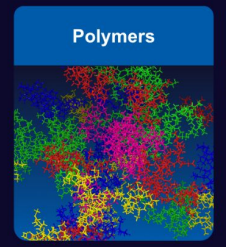


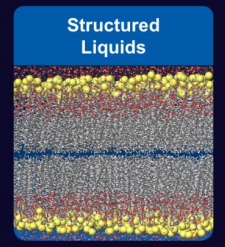


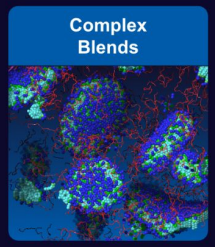


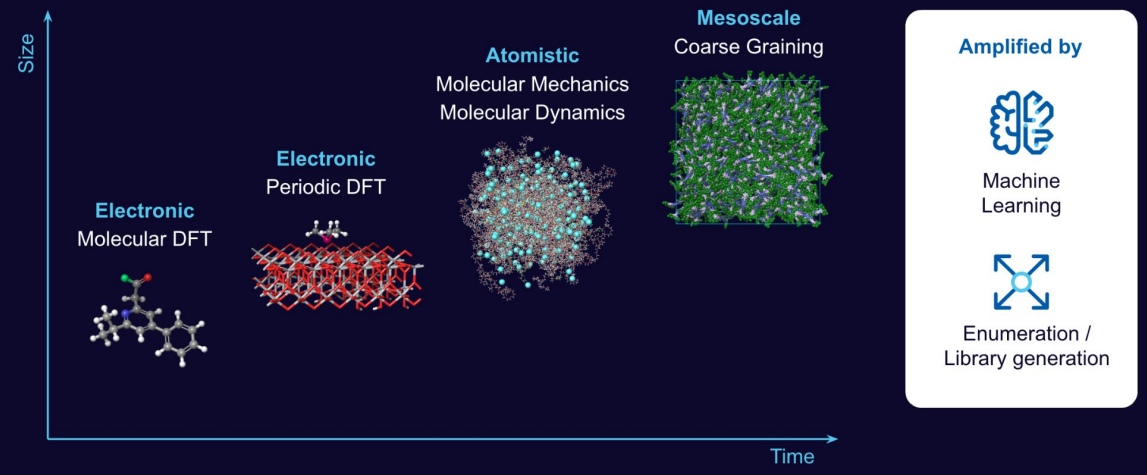








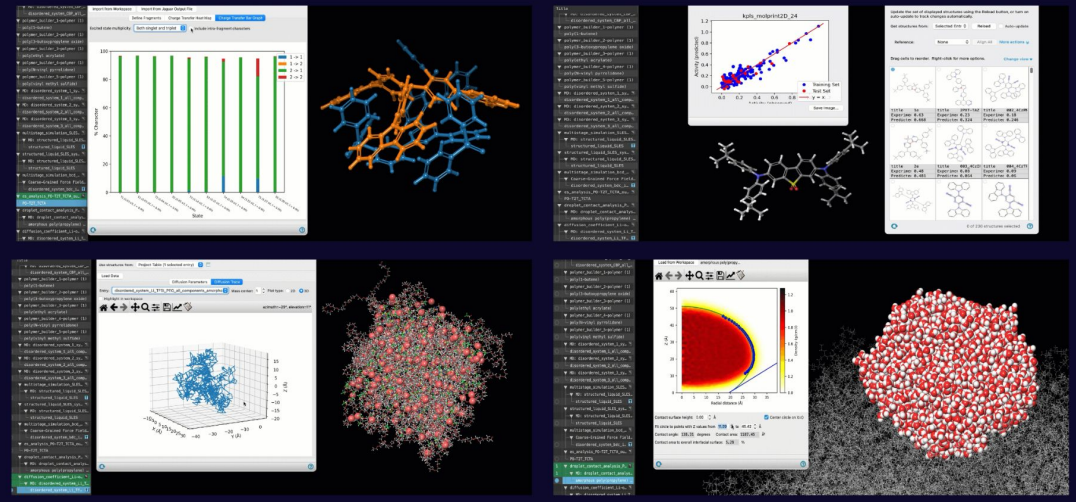




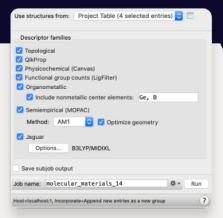
Amplified by

Machine Learning

Enumeration / Library generation



Machine learning

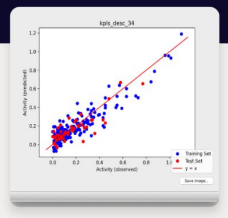


Featurize

Generate extensive descriptors for all classes of materials

Build Models

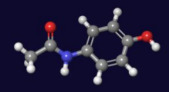
HPC-supported, automated model-building



Predict

Use top model or consensus prediction on unseen systems

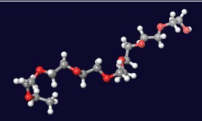
Capabilities for: small molecules, organometallics, polymers, periodic inorganics, and formulations



Small molecules

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

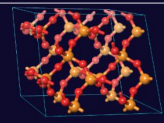
Physics-based descriptors:
- Quantum mechanics
- Auto Reaction Workflow



Polymers

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

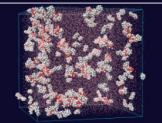
Physics-based descriptors:
- Molecular dynamics
- Quantum mechanics



Periodic inorganic solids

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

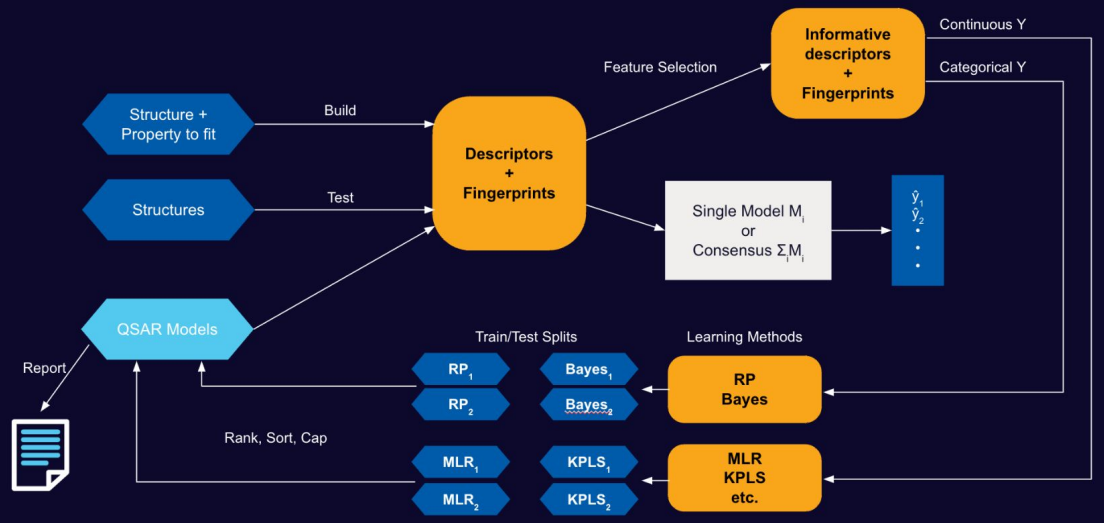
Physics-based descriptors:
- Periodic quantum mechanics



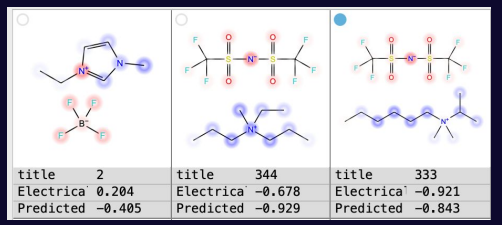
Formulations and mixtures

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

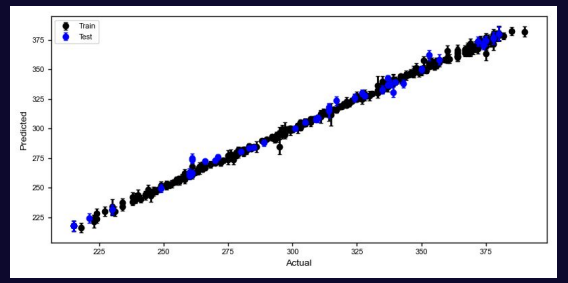
Physics-based descriptors:
- Molecular dynamics

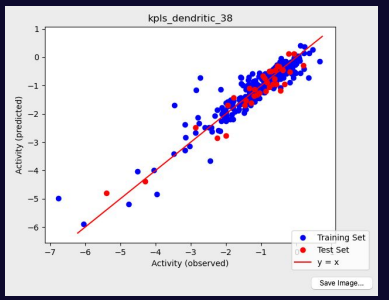


Model Code	Score	S.D.	R^2	RMSE	Q^2	Q^2 MW (Null
kpls_dendritic_38	0.8590	0.3468	0.8584	0.3451	0.9036	-0.0071
kpls_linear_38	0.8319	0.3664	0.8415	0.3770	0.8849	-0.0071
kpls_linear_40	0.8277	0.4017	0.8216	0.3384	0.8400	0.0146
kpls_dendritic_40	0.8159	0.4099	0.8142	0.3912	0.7862	0.0146
kpls_linear_23	0.8039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





Integrated simulation approaches

Jaguar

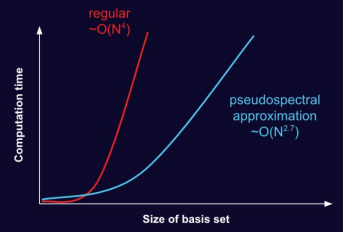
A high-performance quantum chemistry software program leveraging the pseudospectral approximation method

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.

Speed-up (hybrid DFT):

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

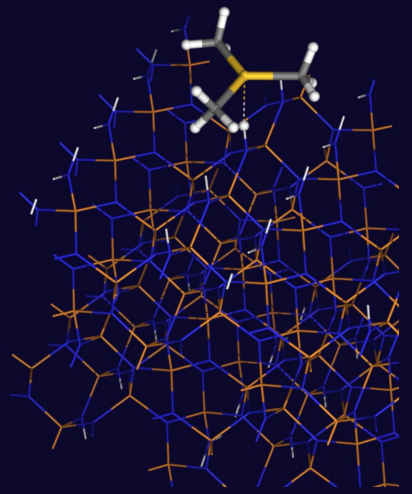


Quantum ESPRESSO

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

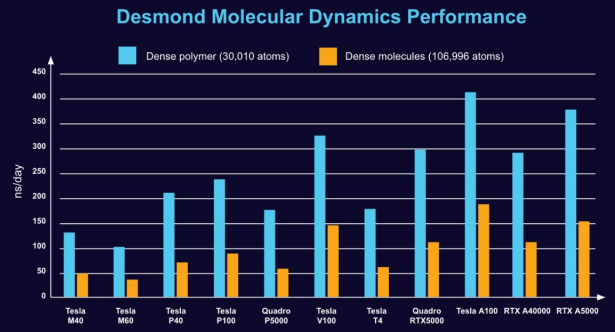


Desmond

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

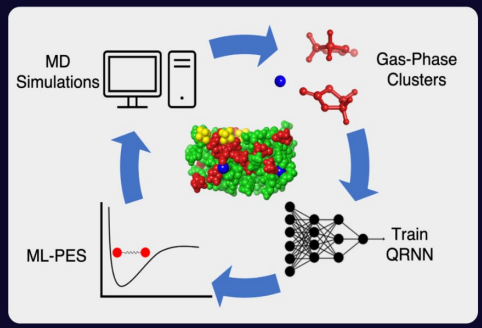


Machine Learning Force Field

Leverage training data from ab initio and classical approaches to generate accurate and fast case-specific force fields

Key capabilities:

- Training data from quantum mechanics (Jaguar, QuantumESPRESSO) and classical molecular dynamics (Desmond)
- Charge recursive neural network (QRNN) architecture
- Validated approach for various materials science applications



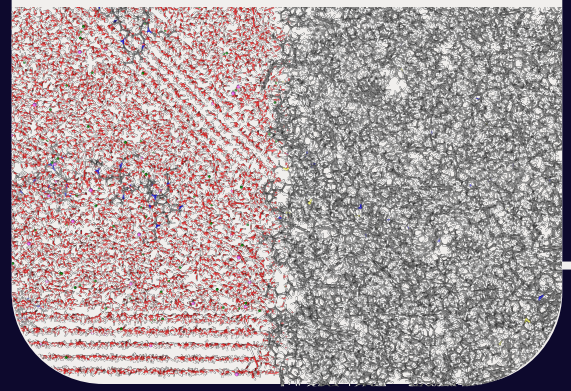
Single platform advantage

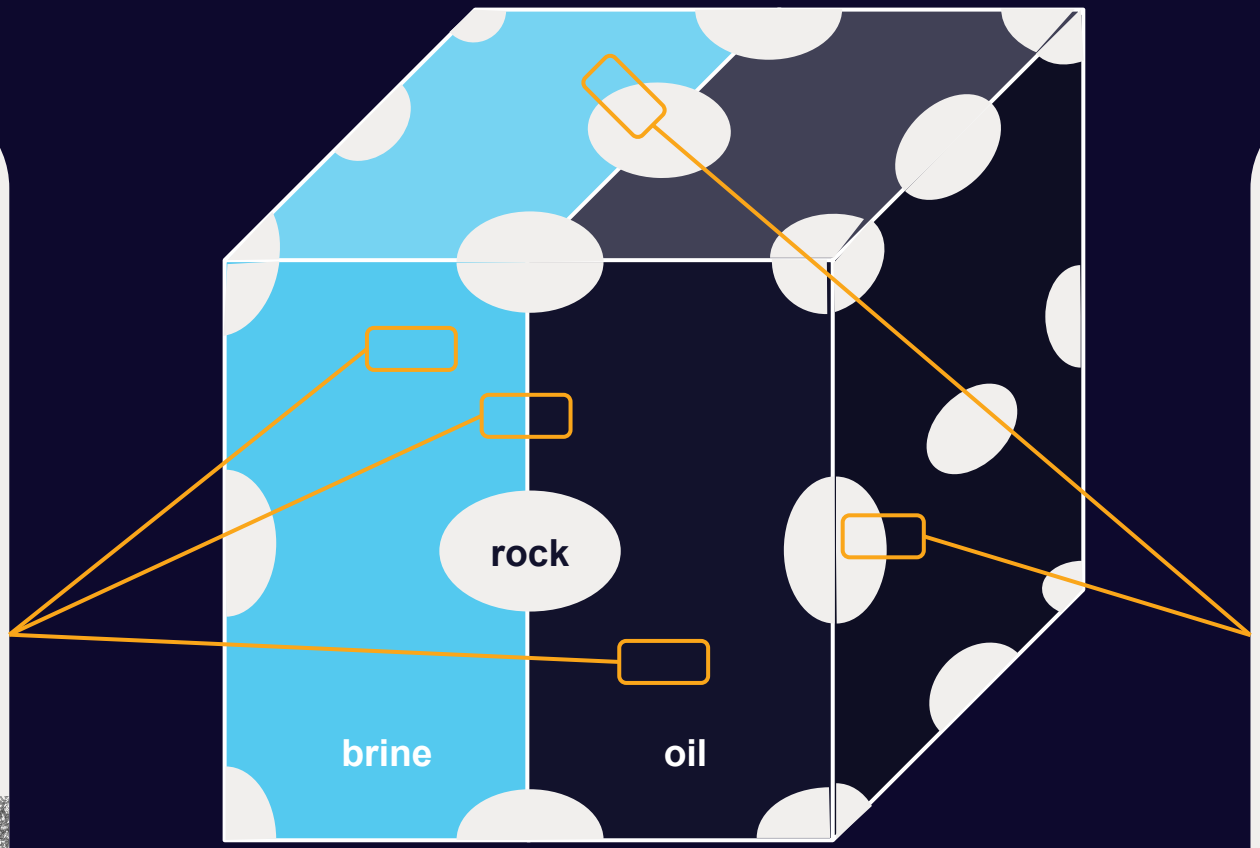
Upstream Modeling Framework

Molecular dynamics and coarse-grained (MD & CG) modeling of brine, oil, and the brine-oil interface

Components: water, salts, hydrocarbons, cycloalkanes, aromatics, olefins, resins, asphaltenes, polymers, surfactants, nanoparticles, etc.

Outputs: energies, forces, morphology, density, interfacial tension, wettability, viscosity, diffusivity





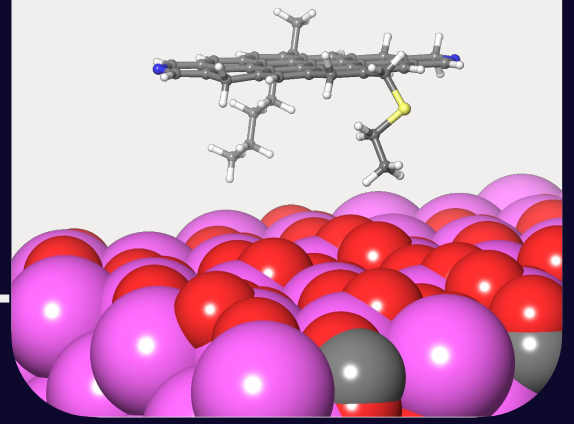
Machine learned force field (MLFF) for comprehensive upstream modeling

'Universal' model with full component coverage of relevant chemical space

Quantum mechanical (DFT & AIMD) modeling of the brine/rock and oil/rock interface

Components: hydrocarbons, cycloalkanes, aromatics, olefins, resins, asphaltenes, rock minerals/scale-forming compounds, etc.

Outputs: energies, forces, bulk and surface properties, reactivity



Brine/oil/rock graphic adapted from: Kirch, A. et al. Multiscale Molecular Modeling Applied to the Upstream Oil & Gas Industry Challenges. Polytechnica 3, 54–65 (2020).

Modeling graphics generated in Schrödinger Materials Science Maestro

Classical simulations

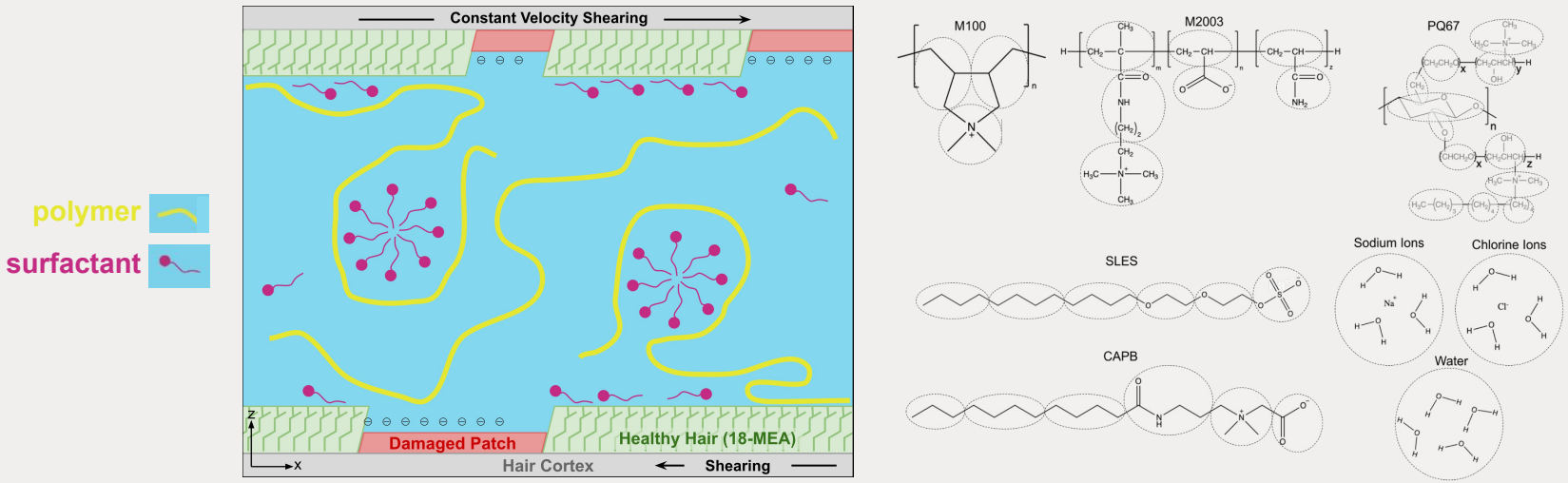
Schrödinger unique advantage:

- Desmond GPU enables large system size and long simulation time
- Out-of-the-box OPLS force field provides excellent materials coverage
- Automated particulation and force field parameterization enables facile linking of molecular and meso-scales

Relevant experience:

- **L'Oreal**: blog, paper
- **AbbVie**: paper, case study
- **Evonik**: white paper
- Internal expertise
- 100+ contract research projects

Schematic from complex coarse-grained approach employed in a surfactant emulsion project



Schematic: Coscia, Benjamin J., et al *Physical Chemistry Chemical Physics* 25.3 (2023)

Quantum calculations

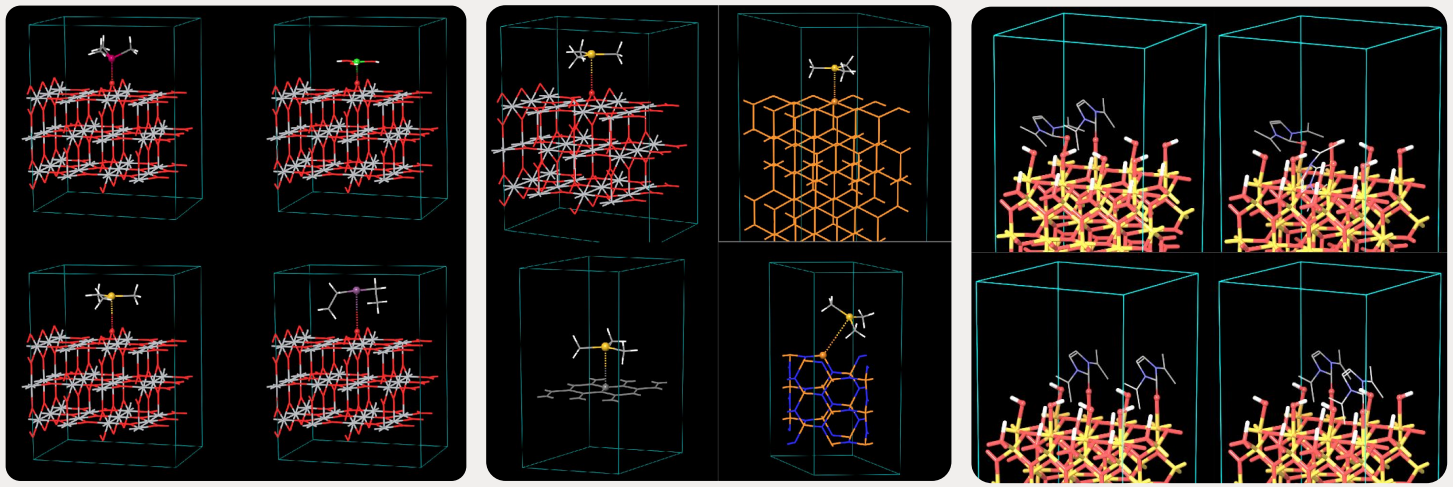
Schrödinger unique advantage:

- Efficient builders for structure generation, slab generation, and adsorbate enumeration
- Extensive experience with at-scale, cloud-based high-throughput quantum mechanical calculations

Relevant experience:

- **Panasonic**: blog, paper
- Public collaborations:
  - **Eonix**: blog
  - **Copernic**: blog
- Internal expertise
- 100+ contract research projects

Rapid adsorbate enumeration capability for high-throughput system building



enumerate adsorbates | enumerate substrates | enumerate binding modes

Machine learned force field

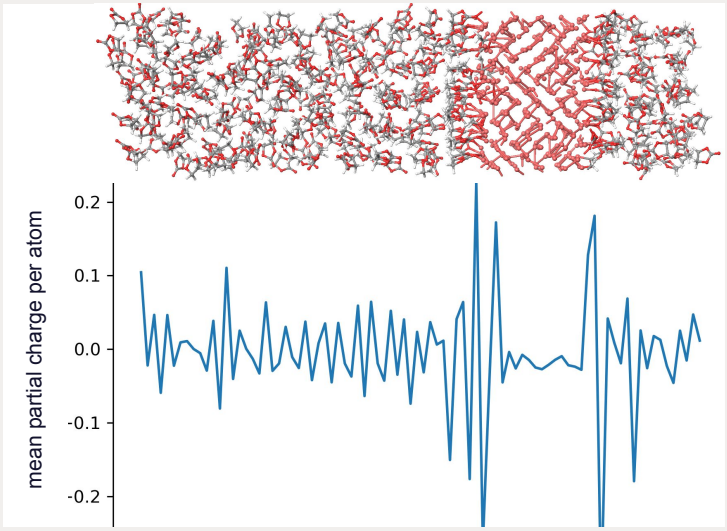
Schrödinger unique advantage:

- Extensive experience developing MLFF, most notably for complex battery materials (solids, liquids and interfaces)
- MLFF community is following our lead for model development (see, e.g., Bytedance AI Molecular BOOster, Csanyi & Grey)

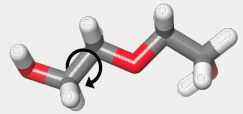
Relevant experience:

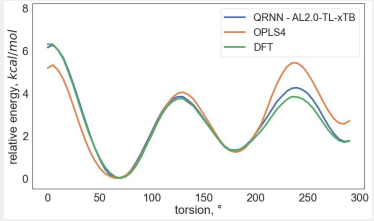
- **Battery Project with Gates Ventures LLC**:
  - Paper
  - Meeting Abstract
- White paper
- Internal expertise

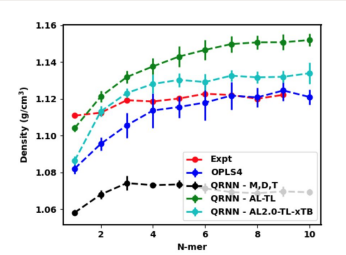
MLFF for Solid-Electrolyte Interphase

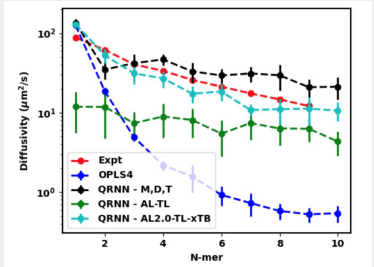


MLFF for Polymeric Materials









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

Contact:
Michael Rauch, Associate Director of Materials Science
michael.rauch@schrodinger.com