Schrödinger

Schrödinger Capabilities for A&D

Schrödinger

Pioneering Digital Chemistry

30+ years of innovation

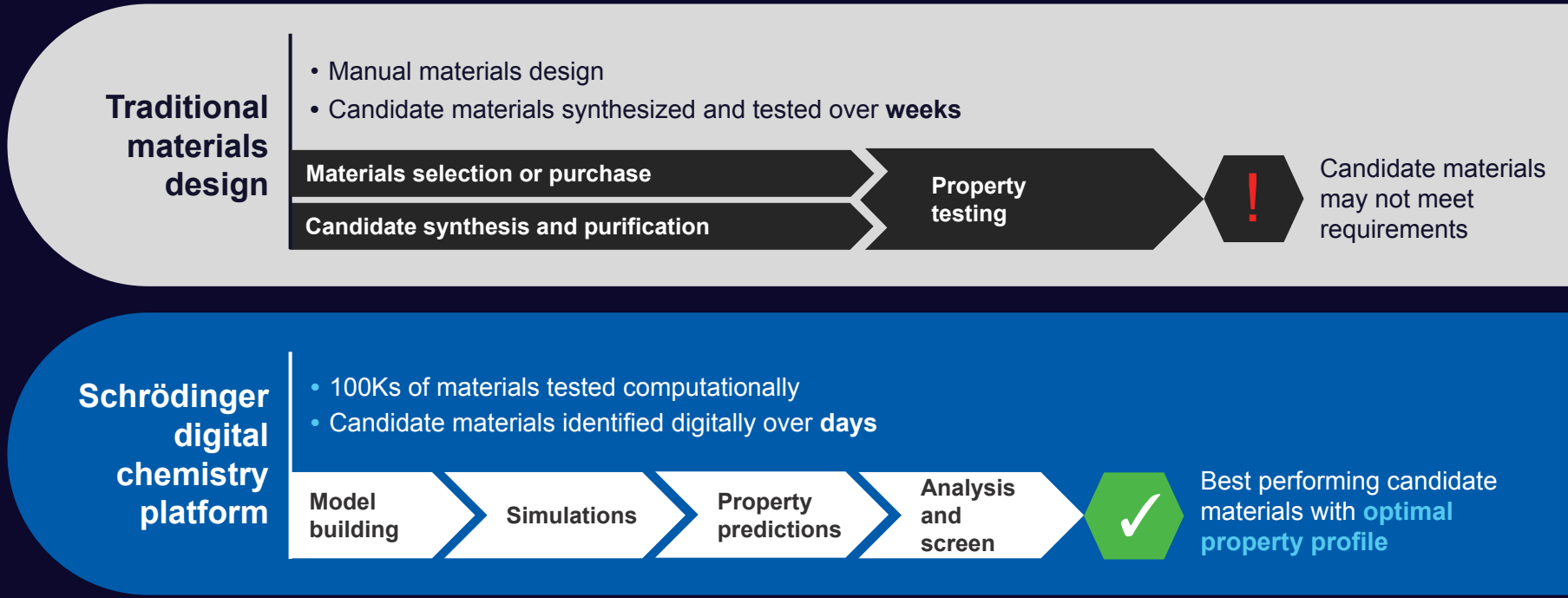
Over 850 employees worldwide; >40% Ph.D.

>50% of employees dedicated to R&D

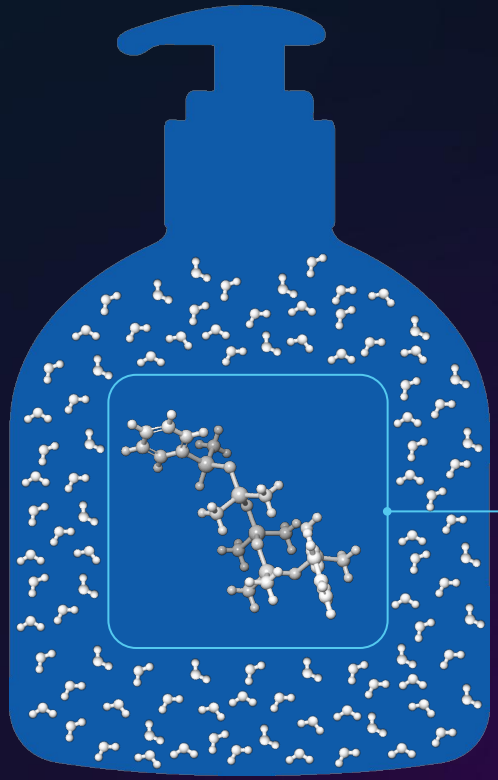
~1,785 customers worldwide

Pipeline of 25+ collaborative and proprietary programs

A predict-first approach



Informed selection

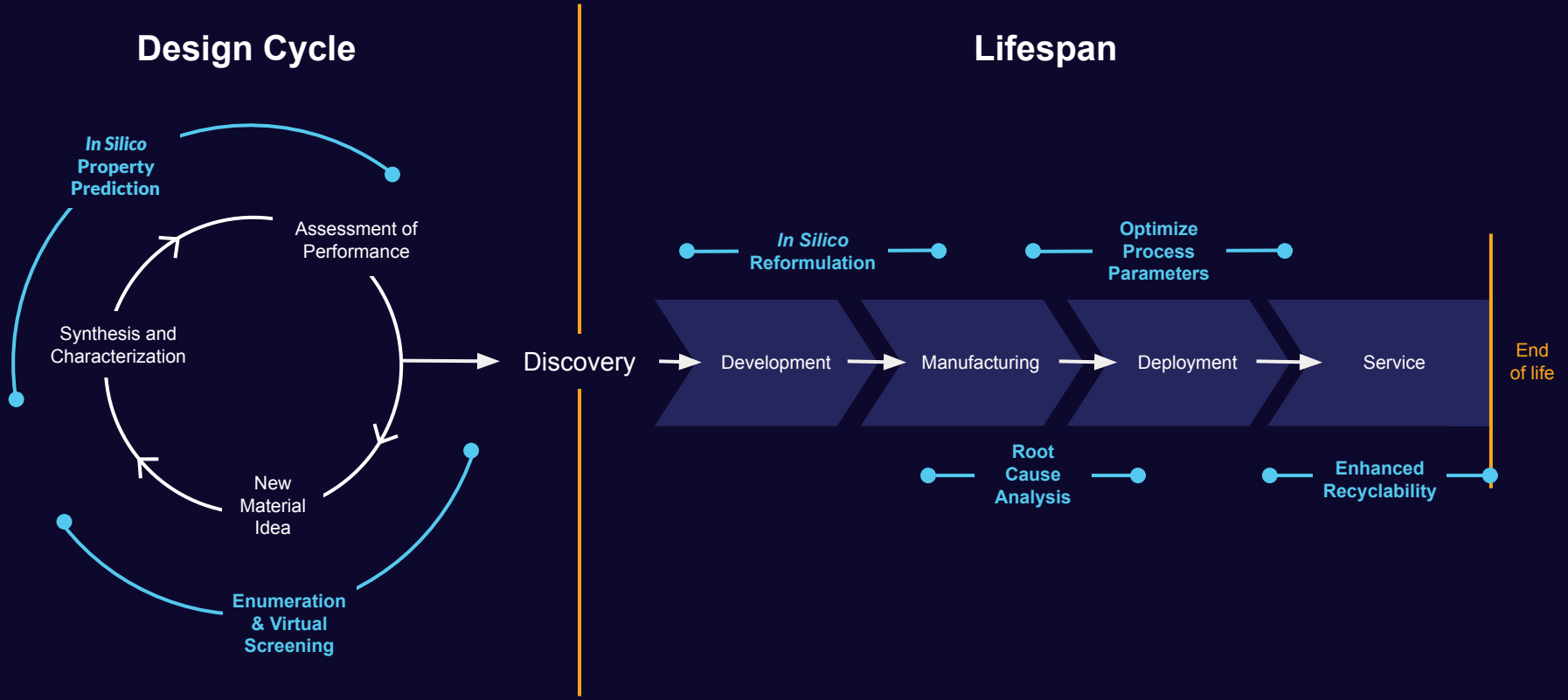


Property / Behavior to optimize, e.g.:

- Miscibility
- Viscosity
- Stability
- Hygroscopicity

Target Property / Behavior

Modeling impact on materials design



Benefits of leveraging digital technology

Less

- **Time** to insights and target solutions
- **Cost** to optimize materials development process
- **Experimental synthesis and testing** of materials with undesirable properties
- **Distance** between teams and expertise areas

More

- **Hypotheses** to test
- **Access** to chemical space
- **Optimization** of multiple property parameters at the same time
- **Dynamic collaboration** in the design process
- **High-quality** materials with desired performance and properties

Synergy between physics-based modeling and machine learning

Physics-based modeling

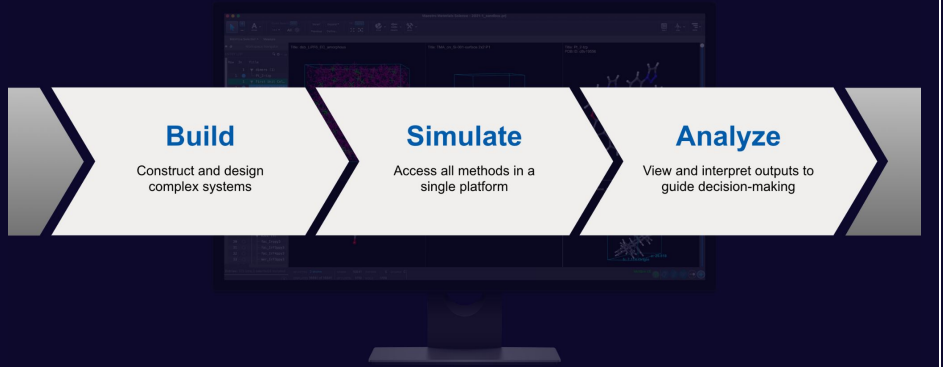
Physics & Machine Learning

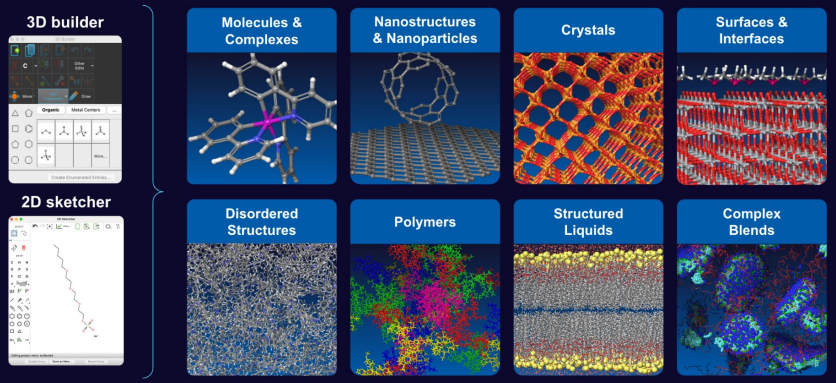
Incorporate physics-based information about materials into practical ML models.

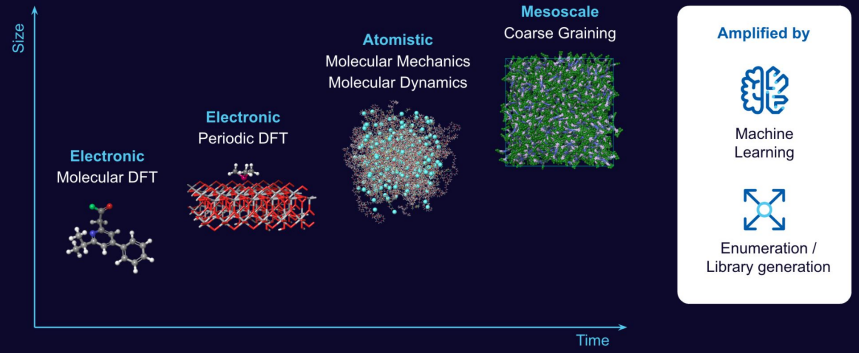
Build targeted ML models to expand the impact of physics-based simulations.

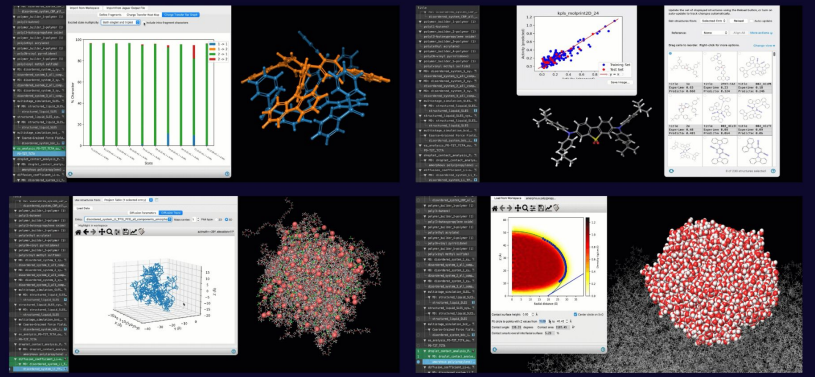
Machine learning

Physics-based modeling









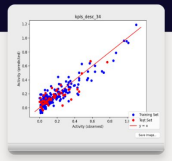
Machine learning

Featurize

Generate extensive descriptors for all classes of materials

Build Models

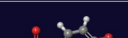
HPC-supported, automated model-building



Predict

Use top model or consensus prediction on unseen systems

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



Small molecules

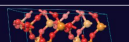
- Physiochemical, topographical descriptors
- Binary fingerprints (RDKit, Canvas)
- Graph-based convolution neural networks

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

Polymers

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

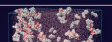
Physics-based descriptors:
- Molecular dynamics
- Quantum mechanics



Periodic inorganic solids

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

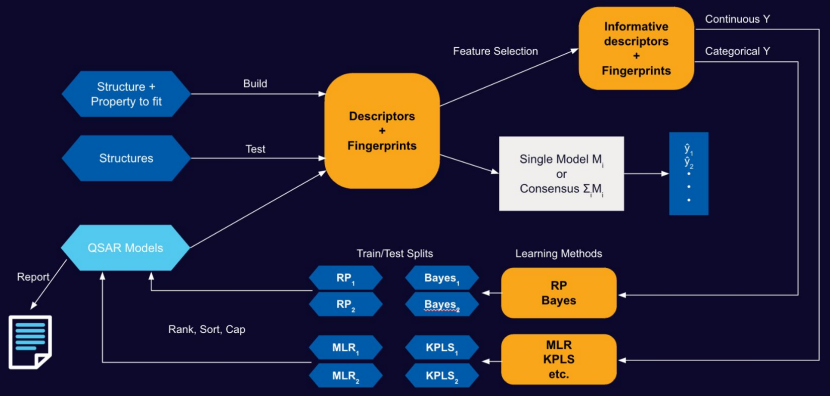
Physics-based descriptors:
- Periodic quantum mechanics



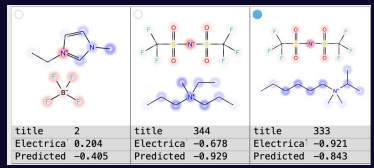
Formulations and mixtures

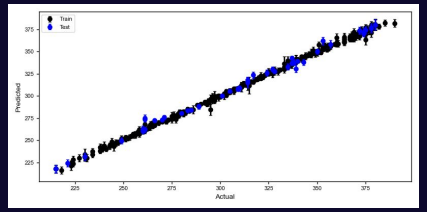
- Composition
- Chemistry of the components
- Experimental/processing conditions

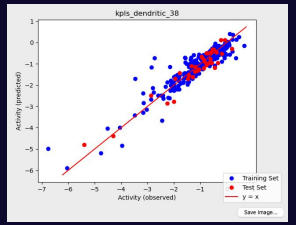
Physics-based descriptors:
- Molecular dynamics



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	0.4004	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

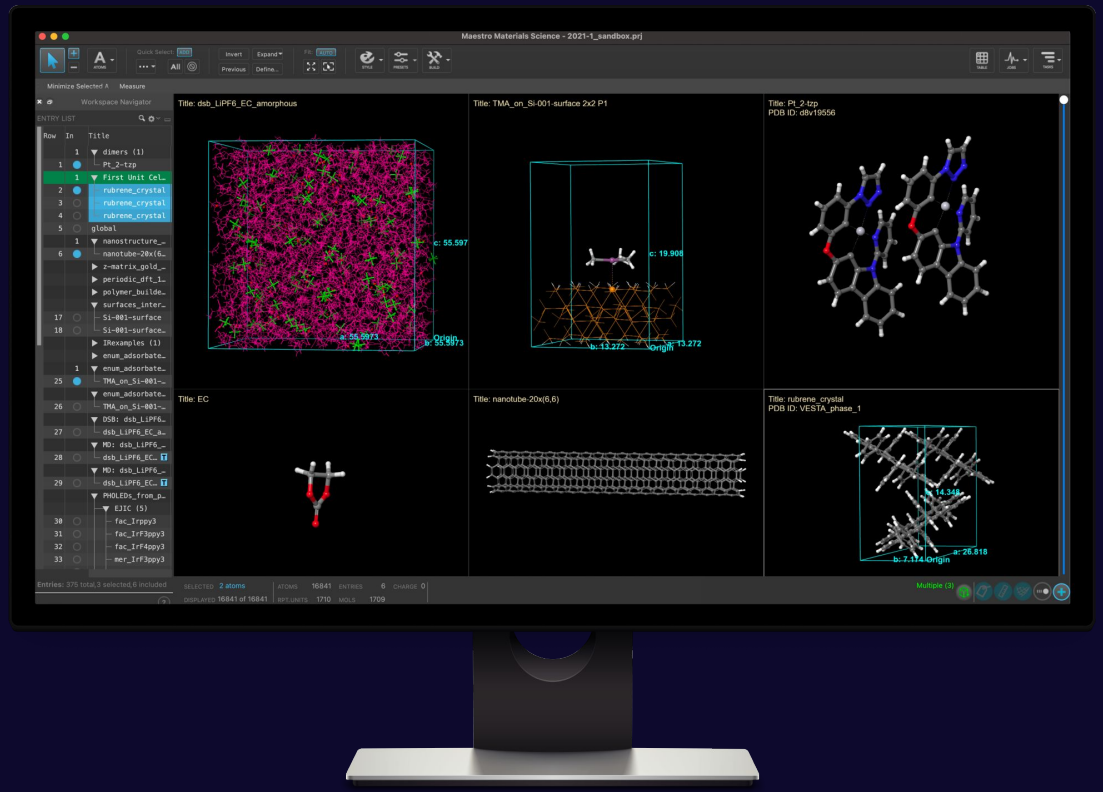






User-friendly GUI and comprehensive API

MS Maestro

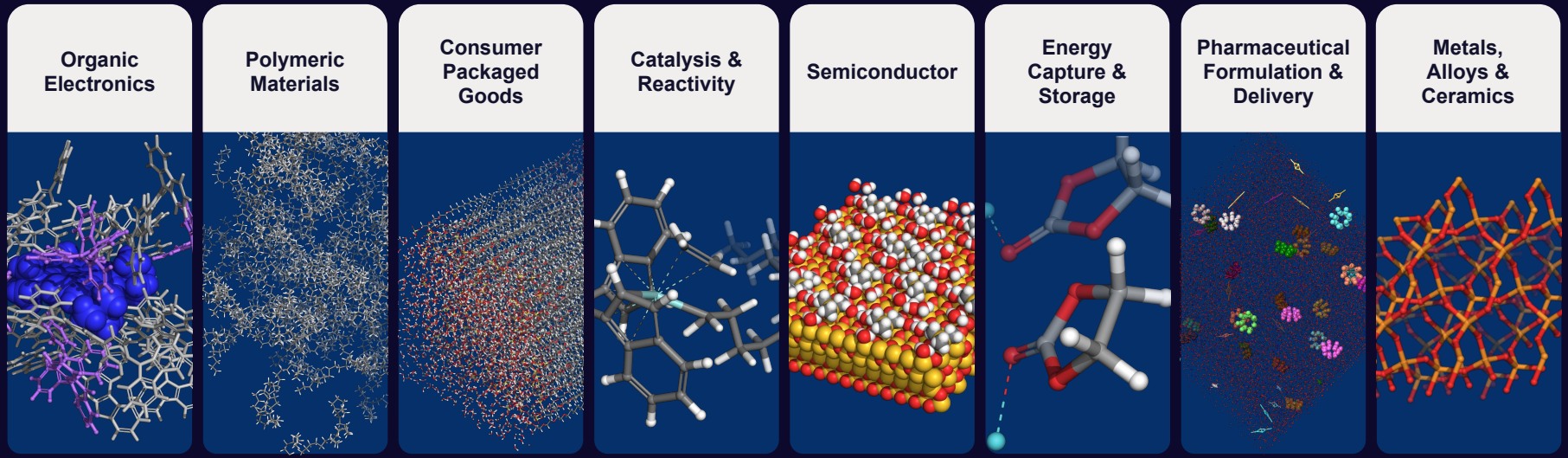


Python API

Comprehensive API for programmatic interaction with Schrödinger software

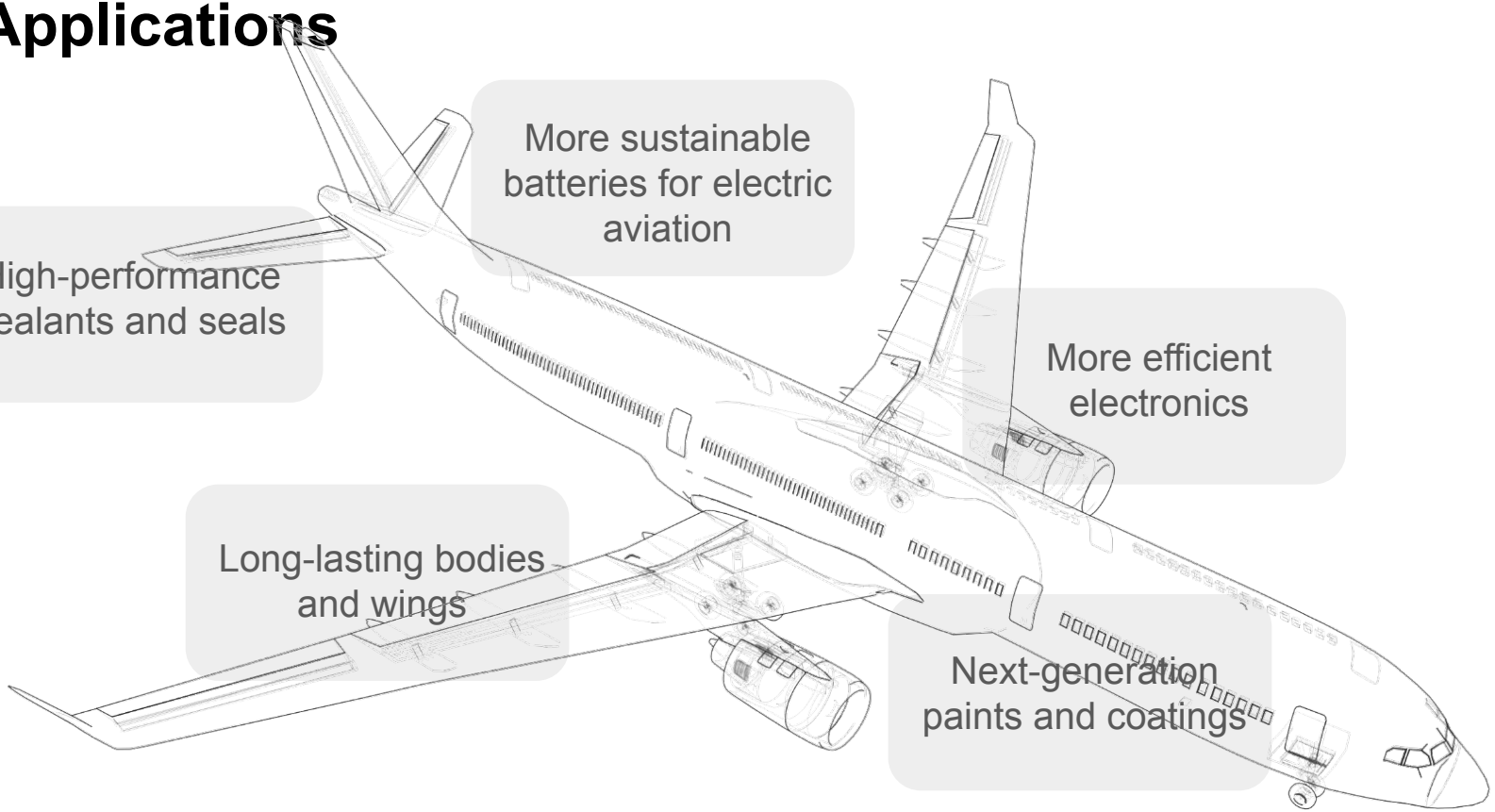
```
➜  ~ export SCHRODINGER=/opt/schrodinger/suites2024-1

➜  ~ $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)
➜  ~
```

Solutions for all applications



Tailored solutions that reduce cost, reduce risk, shorten timelines

A&D Applications



A&D Applications

Composites and ceramics

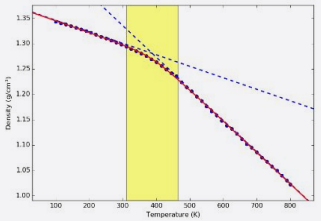
Lubricants, fuel additives, hydraulic fluids

Superalloys

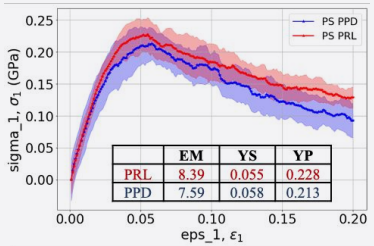
Propellants

Polymeric materials: select capabilities

Glass transition temperature

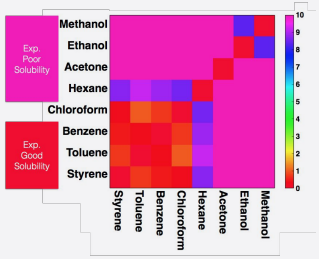


Mechanical response

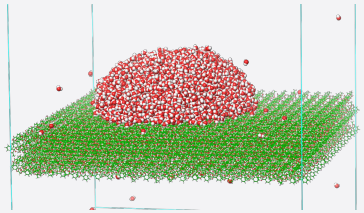


	EM	YS	YP
PRL	8.39	0.055	0.228
PPD	7.59	0.058	0.213

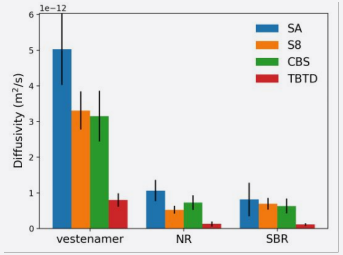
Miscibility and solubility



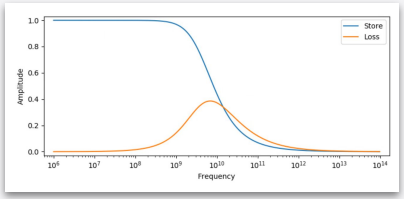
Contact angle



Diffusivity

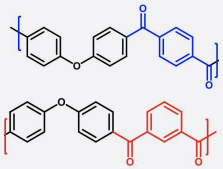


Dielectric properties



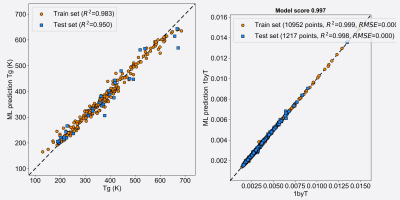
Bond dissociation energy

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



Fast-Tracking Next-Gen Polymers: How SABIC is Leveraging Machine Learning and Physics

“

With the success of this project, we are now inspired in adopting a ‘computation-first’ approach in our current and future projects.

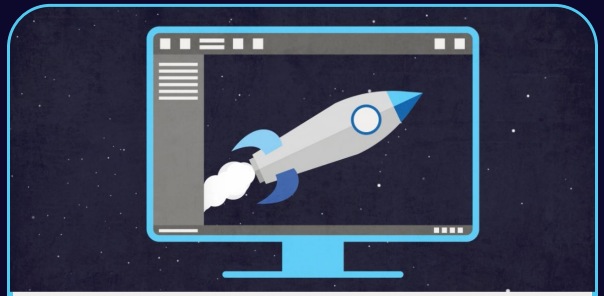
— Vaidya Ramakrishnan, Sabic
— André van Zyl, Sabic

LINK TO BLOG

www.extrapolations.com/fast-tracking-next-gen-polymers-how-sabic-is-leveraging-machine-learning-and-physics/

Uncovering Better Materials for the Spacecraft of Tomorrow

> “The advantage of digital simulation is that it can eventually help cut down on the number of new molecules we’d need to synthesize, leading to a more efficient and less resource-intensive iteration cycle.
>
> — Levi Moore, United States Air Force Research Laboratory



LINK TO BLOG

www.extrapolations.com/uncovering-better-materials-for-the-spacecraft-of-tomorrow/

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

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

Contact:
Jorge Avillez, Materials Science Account Manager
jorge.avillez@schrodinger.com