Hands-On Workshop in nanoHUB: Machine Learning Models for Ionic Conductivity with Schrödinger's AutoQSAR

Dr. Michael Rauch, Materials Science Education Lead, Schrödinger

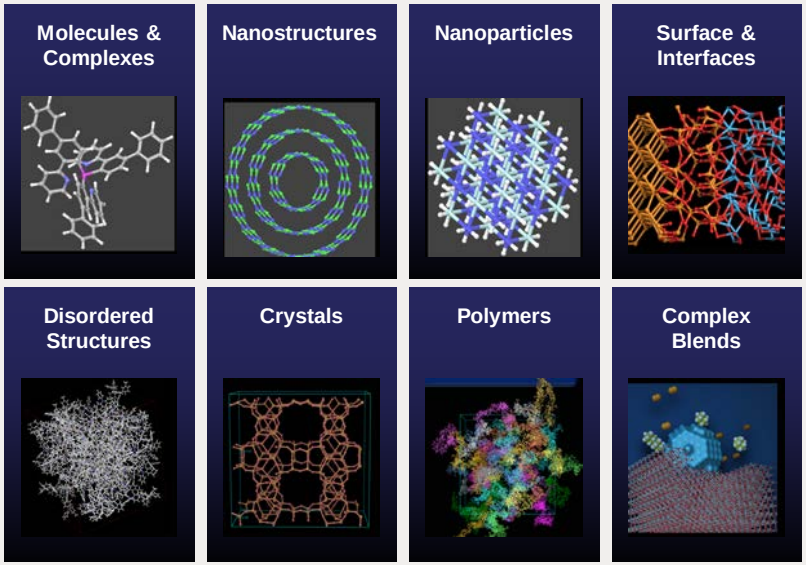
The Schrödinger Platform: An integrated solution for digital materials discovery and analysis

- **A streamlined intuitive GUI** for structural visualization, cutting-edge predictive atomistic simulation and machine learning workflows for Materials Science discovery and analysis.
- **A powerful web-based informatics and molecular design platform** that enables team to rapidly advance materials discovery projects by collaborating, designing, experimenting, analyzing, tracking, and reporting in a centralized platform.

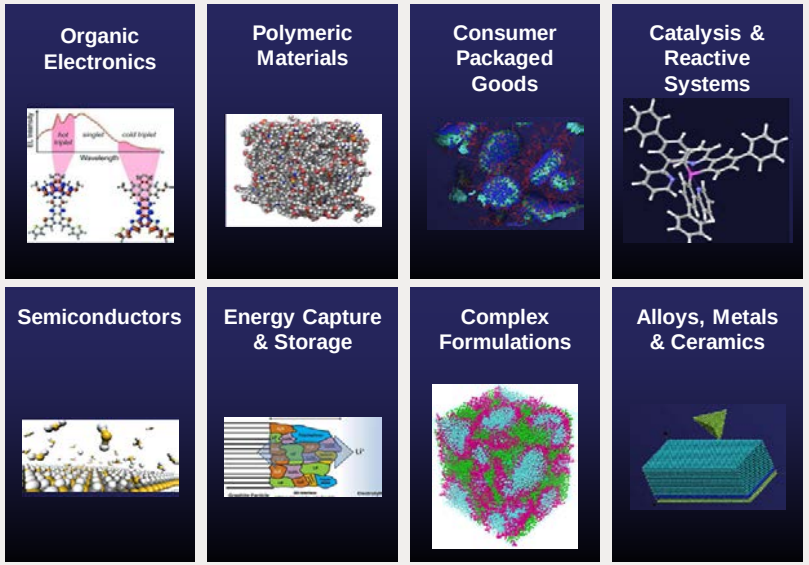
Build advanced models or systems → **Run simulations or automated workflows** → **Predict properties and performances** → **Analyze and Screen** → ✓ **Guide experimental design**

Atomistic Simulation Across Diverse Systems and Applications

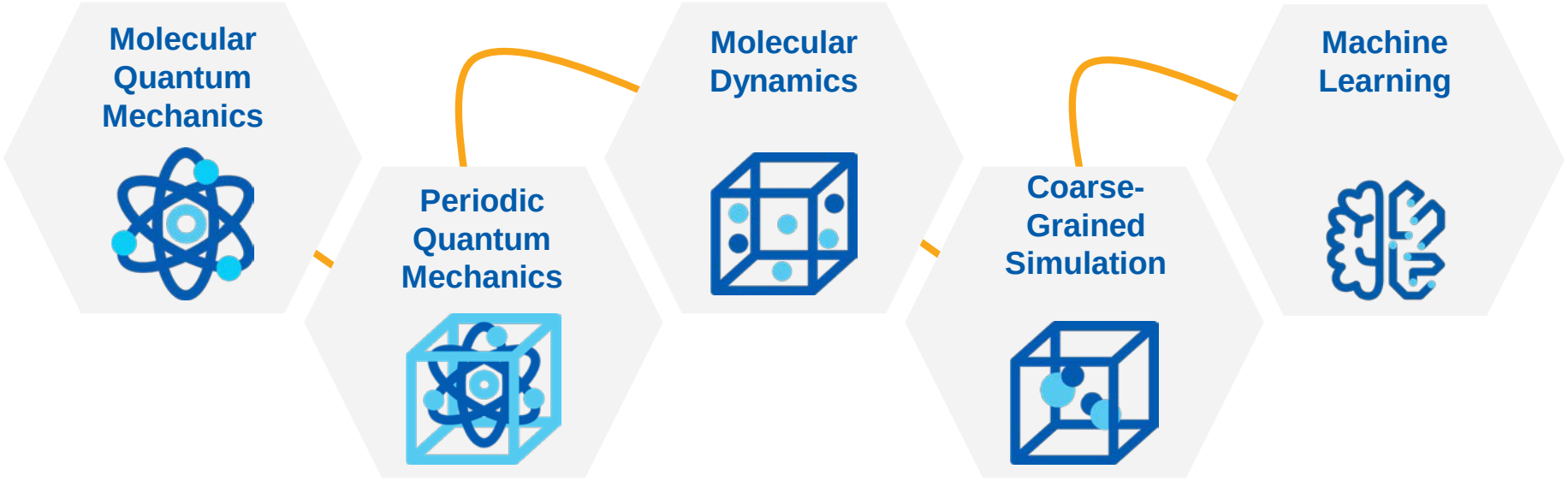
Chemical Systems



Application Verticals



Methods Power Capabilities



From Engines to Workflows

	***Jaguar*** **Molecular Quantum Mechanics**	multistage workflows, optoelectronic properties, automated reaction workflow
	***Quantum ESPRESSO*** **Periodic Quantum Mechanics**	adsorption energy workflows, surface energy, microkinetics
	***Desmond*** **All-Atom Molecular Dynamics**	multistage workflows, thermophysical properties, crosslinking
	***Desmond*** **Coarse-Grained Simulation**	multistage workflows, automated DPD parameterization & Martini mapping
	***AutoQSAR*** **Machine Learning**	materials descriptors, built-in property prediction, active learning

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EXTRAPOLATIONS
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Science & Innovation

SOLVAY

Modernizing the Mining Industry with Digital Simulation

BY ANDREW JACKSON | JAN 18, 2023

Collaborations

reckitt

Driving Sustainability at Reckitt through the Adoption of Molecular Simulations

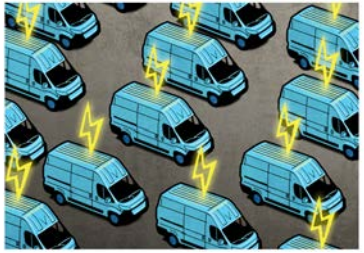
BY MARTIN SETTLE & MARIAM HUSSAIN | MAR 21, 2022

L'ORÉAL

Science & Innovation

How L'Oreal Uses Digital Simulation to Explore Sustainable Product Ingredients

BY SCHRÖDINGER EDITORIAL TEAM | MAY 31, 2023



SEPION TECHNOLOGIES

Science & Innovation

Combating Climate Change with Next-Generation Batteries

BY JESSICA GOLDEN | JAN 24, 2023

U.S. AIR FORCE

Science & Innovation

Uncovering Better Materials for the Spacecraft of Tomorrow

BY SCHRÖDINGER EDITORIAL TEAM & LEVI MOORE | APR 24, 2023

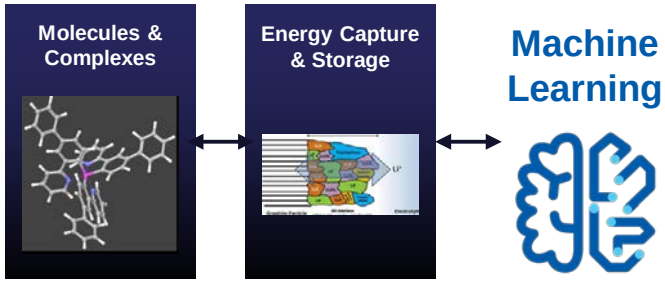
CAMBRIUM

Science & Innovation

Beyond AI: The Importance of Physics-Based Simulations in Sustainable Biomaterials Design

BY PIERRE SALVY, PH.D. & JEFFREY SANDERS, PH.D. | JUN 28, 2023

Today’s Example

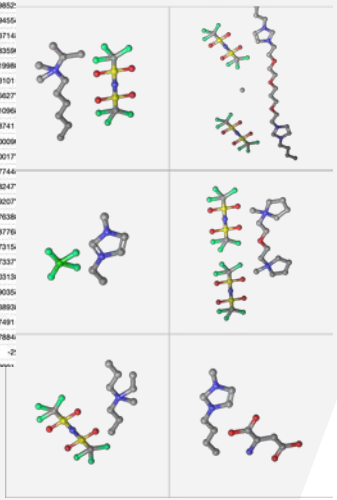


Schrödinger | nanoHUB

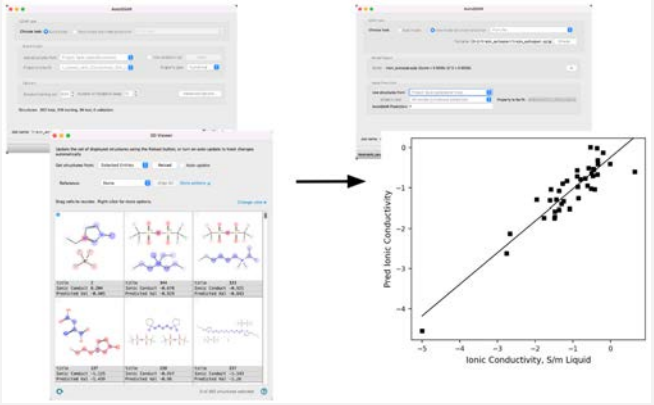
Today's Example

ML Data Input

Index	SMILE	Temperature, K	Ionic Conductivity, S/m Liquid
2	F[B-](F)(F)F.C(C[N+]1=CN(C=C1)C	298.15	0.204459143
344	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F.C(C[N+](CCC)(CCC)C	308.1	-0.677780705
333	FC(S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F)(F)F.C(C(C[N+](CCCCCC)(C)C	295.1	-0.920818754
137	N[C@@H](C)C(=O)[O-].CCC(=O)O.C(CCC[NH+]1CN(C=C1)C	298.15	-1.124938737
238	FC(S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F)(F)F.O(CC[N+]1(CCCC1)C)CC[N+](1	298	-0.91721463
237	C(COCCOCCOCCOC[N+]1=C[N](C=C1)CCC[N+]2=C[N](C=C2)CCOC.	298	-1.142667504
387	F[B-](F)(F)F.C(C[N+]1=CN(C=C1)CCCCCC	298.1	-0.8569852
138	S(=O)(=O)(OC[O-].C(CCC)[N+]1=CN(C=C1)C	298.15	-0.899629455
223	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F.C(CCC[N+]1(CCCCC1)C	298.15	-0.679853714
109	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F.C(CCCCCCC)[N+]1=CN(C=C1	298.15	-0.876148359
150	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F.[NH+]1=CC=CC=C1.C(CCC)#I	303	-0.838631998
11	F[B-](F)(F)F.C[N+]1=CN(C=C1)CCCCCCC	298.15	-1.232473101
27	F[B-](F)(F)F.C(CC[N+]1=CC=CC=C1	298.15	-0.396855627
47	FC(S(=O)(=O)N(S(=O)(=O)C(F)(F)F)F)(F)F.C(CCC[N+]1=CC(=CC=C1)C	298.15	-0.565431096
331	FC(S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F)(F)F.OCC[N+](C(C)C)(C)C	295.1	-0.823908741
376	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F.C(CCCCCCC[N+](C)C)C	298.1	-1.397940009
381	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F.C(CCC[N+](CCCCCC)(CCCC)	298.1	-1.795880017
194	[N-](C#N)C#N.C(CC[N+]1=CC=CC=C1	298.15	0.116607744
183	C(CC)(=O)[O-].C(CCC[N1C[NH+](C=C1)C	303.15	-1.153168247
63	[N-](C#N)C#N.C(C[N+]1=CN(C=C1)C	298.15	0.459249207
16	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F.C(C[N+](CCCCCC)(C)CC	298.15	-1.0520763
148	FC(S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F)(F)F.C(C[P+](CCOC)(CC)CC	298.15	-0.415668776
286	[N-](S(=O)(=O)C(F)(F)F)C(F)(F)F)S(=O)(=O)C(F)(F)F.C(CCCCCCC[N+	295.1	-0.958607315
6	F[B-](F)(F)F.C(CCC[N+]1=CN(C=C1)C	298.15	-0.453457337
81	[N+](=O)([O-])[O-].CN1C=N[N+](=C1)CCC	298.2	-0.745210313
163	FC(S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F)(F)F.C(C)OCN1C=[N+](C=C1)C	298.15	-0.412289035
8	CC1=CC=C(C=C1)S(=O)(=O)[O-].C(C[N+]1=CN(C=C1)C	298.15	-1.062983893
384	P(=O)(OCC)(OCC)[O-].C(C[N+]1=CN(C=C1)C	298.1	-1.045757491
21	F[P-](F)(F)(F)(F)F.C(C[N+]1=CN(C=C1)C	299.1	-0.29627884
338	FC(S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F)(F)F.OCC[N+]1(CCCC1)C)CO	295.1	-2

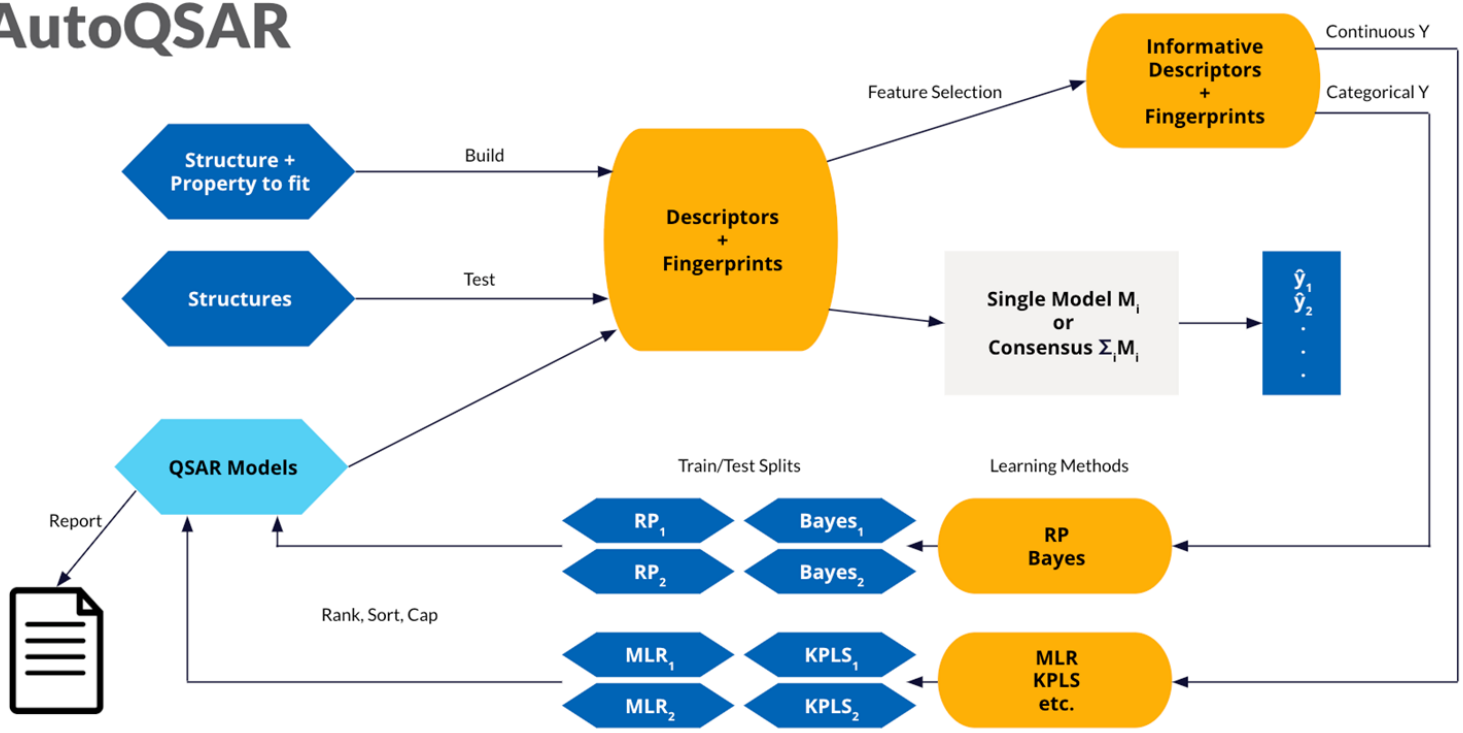


Model Generation and Application



Conductivity prediction model for ionic liquids using machine learning. DOI:10.1063/5.0089568

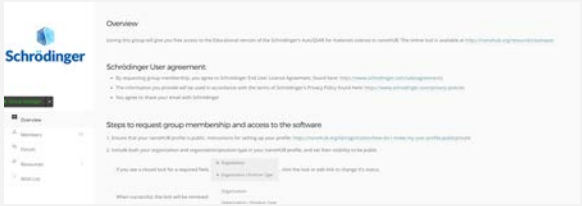
AutoQSAR



nanoHUB Access

Login to nanoHUB and request to join the Schrödinger group

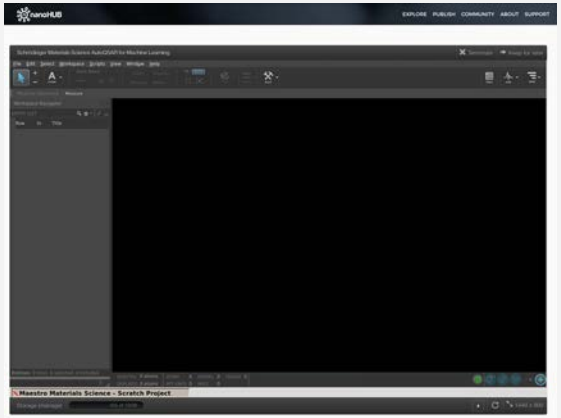
https://nanohub.org/groups/schrodinger



Go to Schrödinger Materials Science AutoQSAR for Machine Learning tool

https://nanohub.org/tools/autoqsar

Launch the Tool and Accept the EULA



Live Demo

Next Steps

Continue Exploring Schrödinger Materials Science Through nanoHUB

Two other datasets are available in nanoHUB for widespread educational use (thermally activated delayed fluorescent materials & homogeneous catalysts)

Learn All Capabilities with Comprehensive Online Certification Courses

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Questions?
Thank you!