APPLICATION NOTE

Machine Learning Force Fields for Improved Materials Modeling

Machine learning force fields (MLFFs), also known as machine learning interatomic potentials, represent an intermediate between classical force fields and density functional theory (DFT), maintaining the linear scaling of the former while approaching the accuracy of the latter. Beyond the balance of accuracy and efficiency/cost, MLFFs are enabling new scientific insights by making large-scale and long-time scale simulations feasible for reactive systems. This opens the door to modeling complex materials systems that were previously computationally prohibitive with traditional quantum methods.

Message Passing Network with Iterative Charge Equilibration (MPNICE) is an MLFF architecture developed by Schrödinger for which multiple pre-trained models spanning 89 elements are available, and which explicitly incorporates equilibrated atomic charges and long range electrostatics.[1] This technological advancement has removed the drawback of previous MLFFs that were limited by the number of unique atomic elements they could model. Furthermore, inclusion of atomic charges and electrostatics through charge equilibration has enabled representation of multiple charge states, ionic systems, and electronic response properties, while simultaneously improving accuracy. In addition to MPNICE, the Schrödinger suite also allows users to utilize the Universal Models for Atoms (UMA),[2] developed at Meta. This suite of models offers very high accuracy, includes a model that yields good performance for reaction barrier heights for finite systems, and covers the majority of the periodic table.

By integrating state-of-the-art MLFF methods with high-performance OPLS4 or OPLS5 force fields, as well as advanced DFT and molecular dynamics (MD) engines, Schrödinger offers a uniquely powerful platform for materials simulation — positioning us as the leading partner in advanced MLFF technologies. In this application note, we present case studies from materials-intensive industries, including batteries and catalysis.

Schrödinger

Benefits of MLFF

Near DFT-level accuracy with orders of magnitude reduction in computational time

Option for GPU accelerated molecular dynamics with Desmond

Large chemical space spanning 89 elements

Specialized force fields for organic, inorganic, and hybrid materials

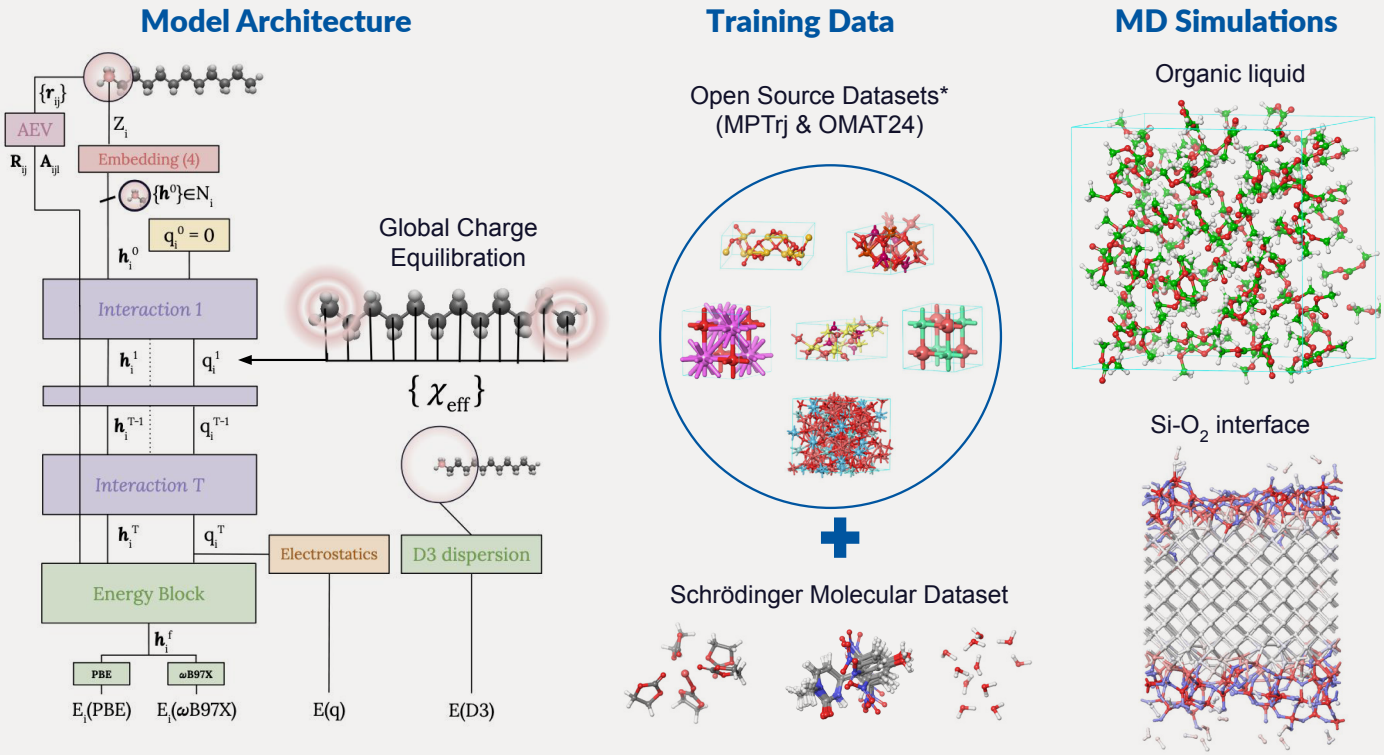


Figure 1: Illustrative examples of Schrödinger's MLFF workflow and its applications

*Datasets references: *Nature Machine Intelligence* 2023, 5, 1031–1041; arXiv:2410.12771

Diverse applications of MLFF

Batteries:

- Calculate bulk and transport properties, such as diffusion, viscosity, and conductivity of liquid electrolytes
- Simulate Li-ion diffusion in solid-state electrolytes and cathode coating materials
- Model electrolyte reactivity and SEI formation

Crystal structure prediction:

- Rank order organic crystal structures

Reactivity in molecules and solid-state:

- Investigate reaction pathways and transition states
- Expedite catalyst design
- Optimize chemical reactions

OLED materials:

- Simulate molecular packing and thin-film morphology
- Investigate doping, host-guest, and interlayer interactions
- Link device properties to the static and dynamic disorder of molecular systems
- Facilitate thermomechanical property prediction
- Model charge and exciton transport

Adsorption on surfaces:

- Study reactivity of multiple adsorbates in extended models of complex surfaces

Polymers:

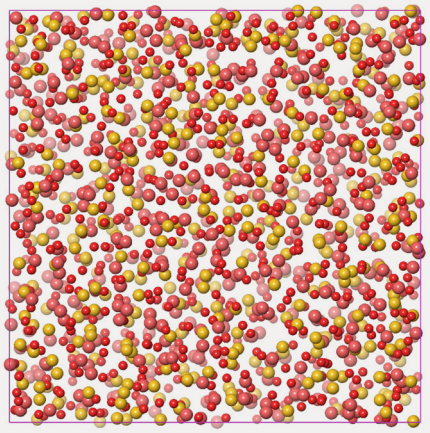
- Evaluate polymer dynamical properties
- Investigate solid polymer electrolytes

APPLICATION

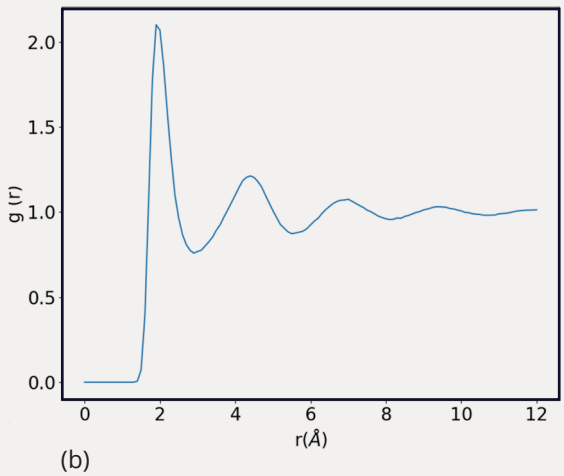
Modeling Li-ion diffusion through inorganic amorphous cathode coating material

Accurate modeling of Li-ion diffusion through inorganic amorphous cathode coating materials was previously challenging due to limitations in time and length scales. Schrödinger's MLFF technology enables accurate prediction of key performance indicators, such as transport of Li-ion diffusion through inorganic coatings. In this example, we demonstrate the application of MLFF to simulate the structure of the amorphous phase of $LiAlO_2$ using a large supercell of 1600 atoms. The amorphous phase was generated using simulated annealing, where the structure is slowly heated above the melting point, followed by equilibration at 300 K and 1 atm for 1 ns using NPT ensemble. We calculated the diffusion coefficient over a wide range of temperatures using large-scale MD simulations and extracted the activation barrier by fitting the Arrhenius equation. The predicted properties showed strong agreement with available experimental data, validating our approach and offering reliable guidance for the design of cathode coating materials in next-generation Li-ion batteries.

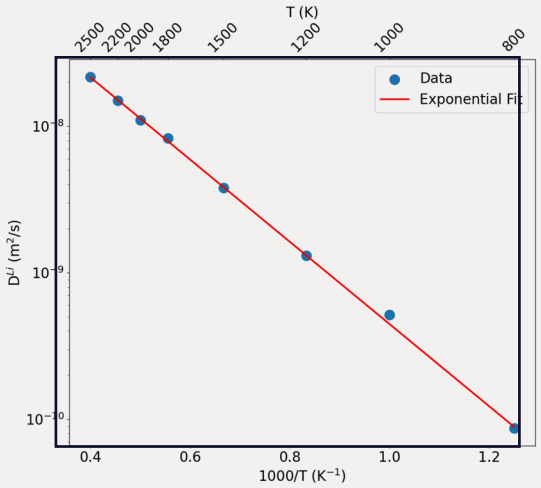
Property	Inorganic MPNICE	Literature
Density (g/cm^3)	2.584	2.615 (Expt)[3]
Coefficient of thermal expansion x 10^{-5} (K^{-1})	5.36	N/A
Activation barrier (eV)	0.55	0.56 (Expt), 0.54 (AIMD)[4]



(a)



(b)



(c)

Figure 2: (a) Equilibrated amorphous structure of $LiAlO_2$ cathode coating material. (b) Li-O radial distribution function (RDF) plot of the amorphous phase. (c) Li-ion diffusivity as a function of inverse of the temperature in amorphous $LiAlO_2$. Activation barrier for Li-ion diffusion extracted by fitting the Arrhenius equation.

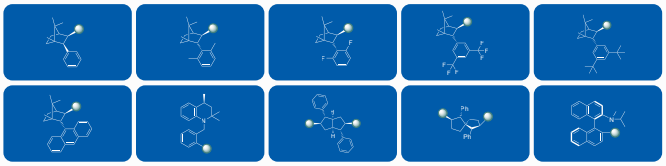
APPLICATION

Virtual high-throughput screening of reactivity with RxnEnumProfiler

RxnEnumProfiler is a fully automated, massively parallel, out-of-the-box workflow developed to systematically evaluate large libraries of chemical species within a fixed reaction topology – that is, a predefined sequence of mechanistic steps involving reactants, products, intermediates, and/or transition states that characterize a catalytic or chemical process. One exemplary application is homogeneous catalyst design, particularly in the context of enantioselectivity screening. For instance, evaluating ten catalysts within a 20 kcal/mol conformer selection window (≈400 transition states) typically requires 1–2 weeks with DFT, assuming immediate access to 2400 CPU cores. In contrast, with delta-learned organic MPNICE tight binding (Organic_MPNICE_TB) the same screening can be completed in about 2.5 hours on 400 cores in a queued system.[1]

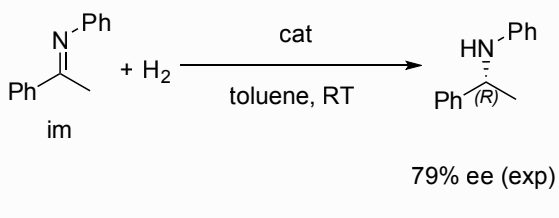
Enantioselectivity screening:

Task scope: Evaluating ten catalysts within a 20 kcal/mol conformer selection window (~400 transition states)

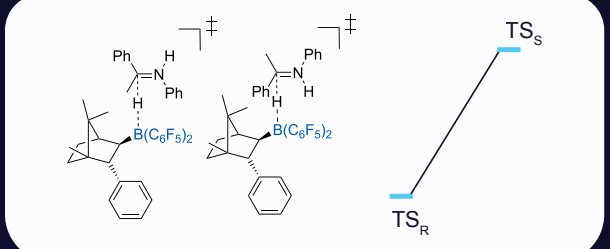


Google Cloud

ωB97X-D/6-31G*//6-311++G**	VS	Organic_MPNICE_TB
2400 cores HPC		400 cores HPC
~1-2 weeks*		2h24m49s



(a) Asymmetric hydrogenation reaction



(b) Reference network for enantioselectivity prediction

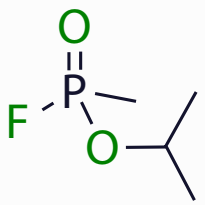
APPLICATION

Optimizing transition state, minima structures, and IRC path for thermal decomposition of sarin with AutoTS

A transition state (TS) represents the highest-energy point along the minimum energy path between reactants and products. Knowing the TS is crucial because it defines the reaction barrier, which directly determines the reaction rate. Schrödinger's AutoTS is an automated workflow for locating transition states for elementary reactions. In addition to DFT and semiempirical potentials, machine learning potentials can now be used in AutoTS for some reaction types.

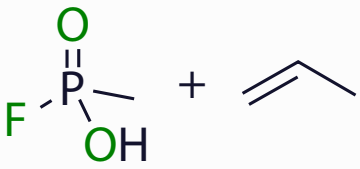
Input: molecular representations for reactants and products (XYZ, SMILES etc)

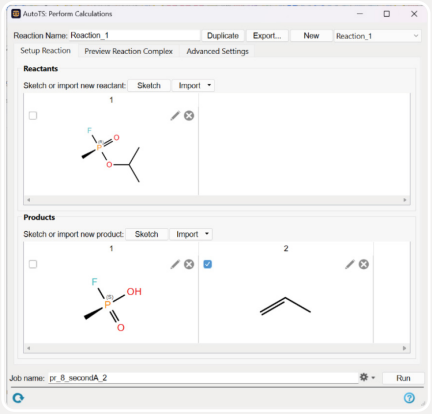
Reactants



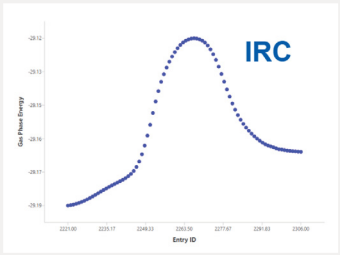
Organic_MPNICE_TB

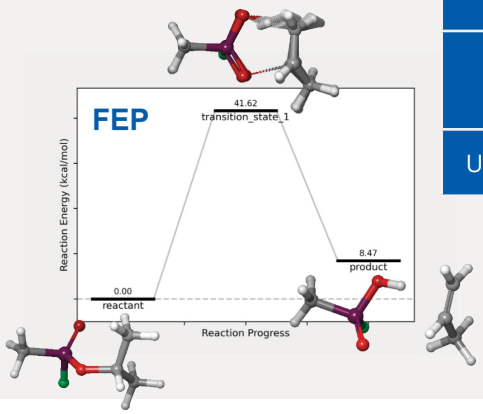
Products





Output: optimized transition state and equilibrium structures, Free Energy profile, IRC profile





Method	# of cores	walltime	ΔG_r (kcal/mol)	$\Delta G^{\ddagger}$ (kcal/mol)
M06-L/6-31G*	8	~ 3 hrs	10.8	35.1
GFN2-xTB	1	~ 6 min	21	41.3
Organic_ MPNICE_TB	1	~ 8 min	8.5	41.6
UMA_sm_omol	1	~ 1 hr	5.3	36.2

Key products

MS Force Field Applications

Cutting-edge force field technologies for accurate property predictions – including OPLS4, OPLS5, MPNICE, and UMA.

AutoTS

Automatic workflow for locating transition states for elementary reactions.

MS Reactivity

Automated workflows for design, optimization, and unsupervised mechanism discovery in molecular chemistry – including RxnEnumProfiler.

References

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4. Ultrathin lithium-ion conducting coatings for increased interfacial stability in high voltage lithium-ion batteries. Park, JS, et al. Chemistry of Materials 2014, 26, 3128–3134.

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