Next-Gen Battery Design: Harnessing the Power of Amsterdam Modeling Suite and Machine Learning

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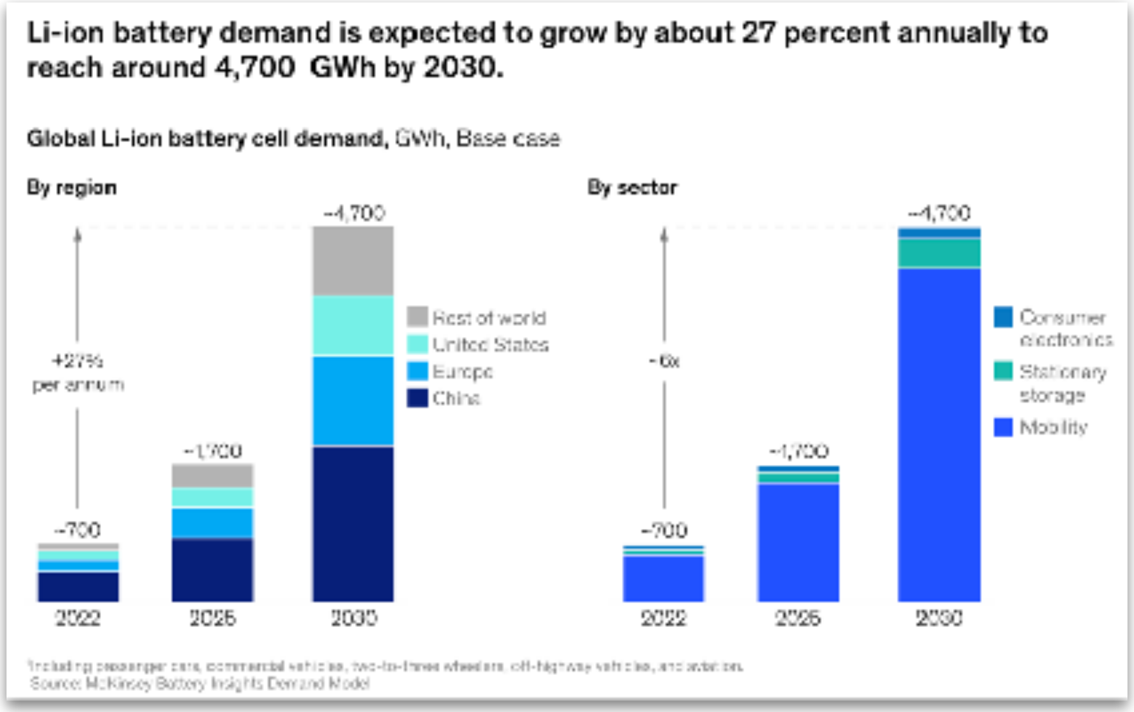
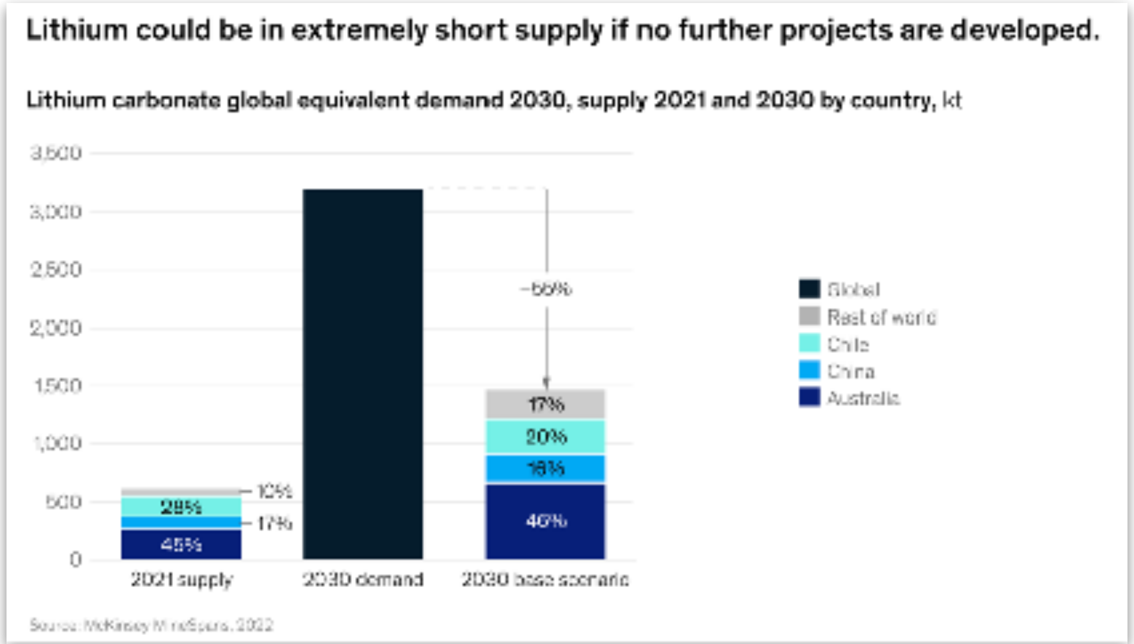
Motivations

Accelerate R&D with modeling

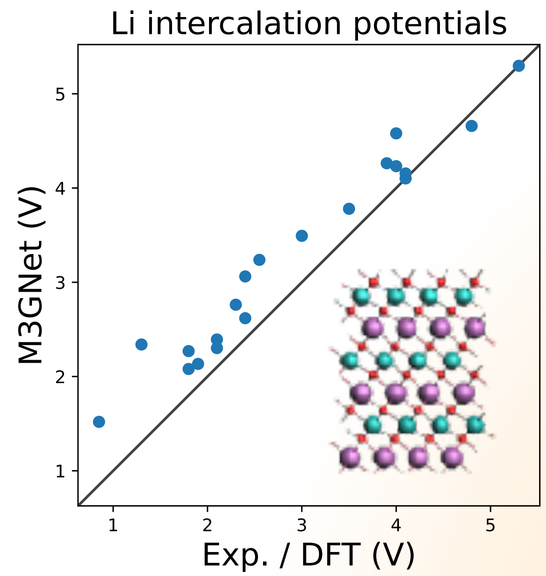
- Battery forecast
  - 400 $billions (2030)
- Challenges
  - Materials shortage
  - Capacity (performance, longevity)
  - Safety, sustainability
- Key to modeling solutions
  - Reduced time-to-market
  - Lower development costs
  - Improved design safety

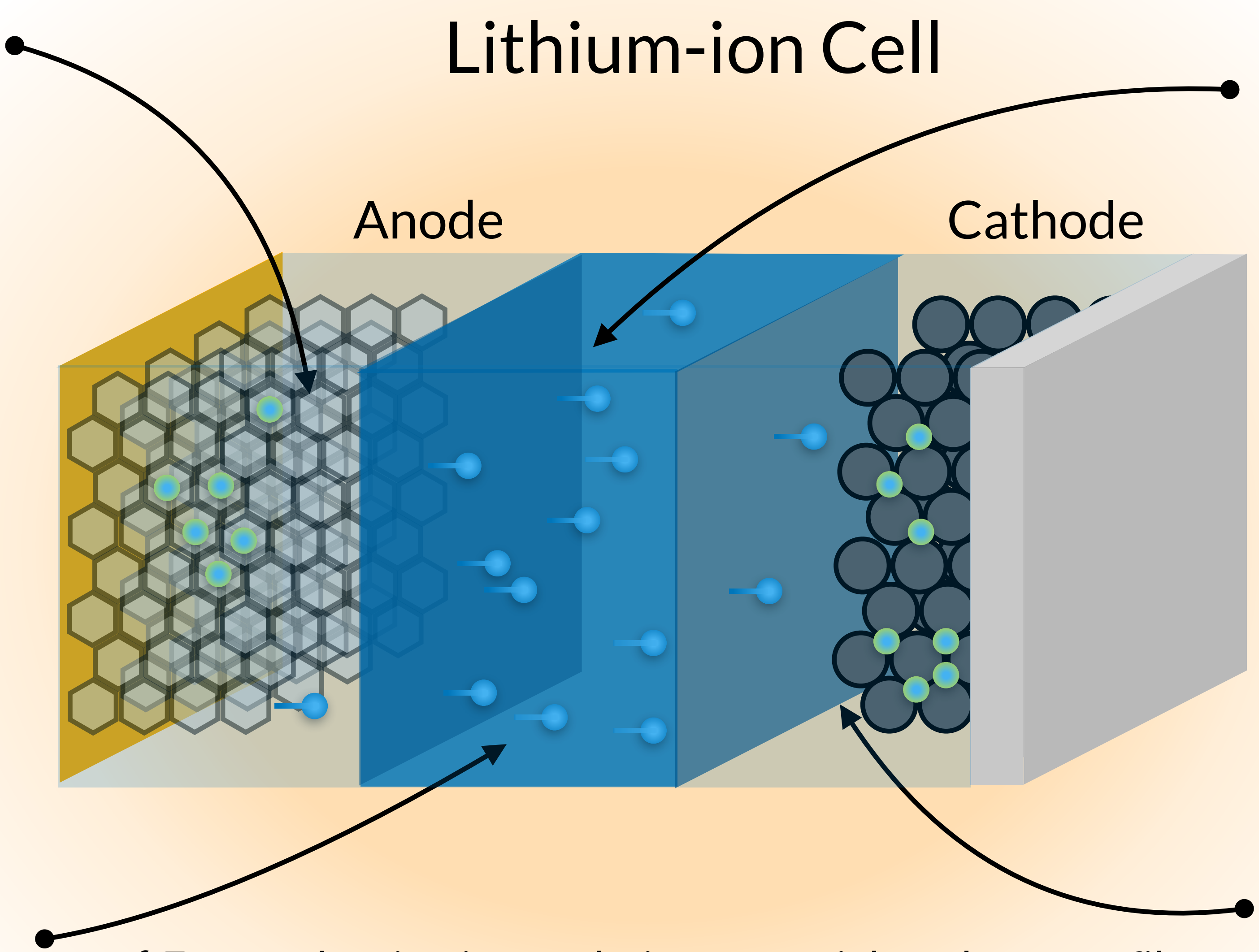


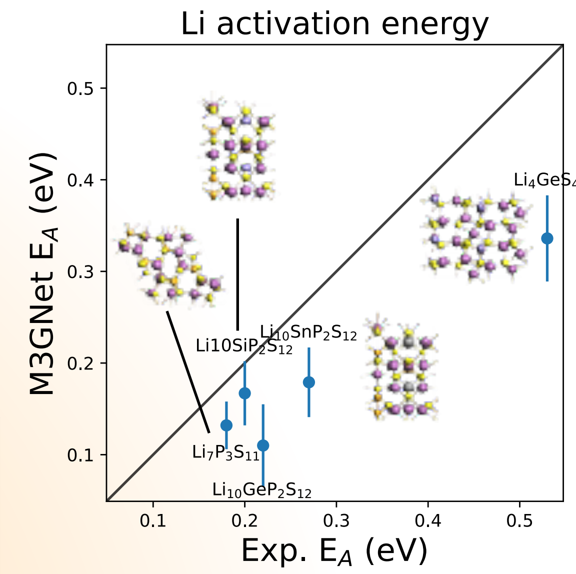


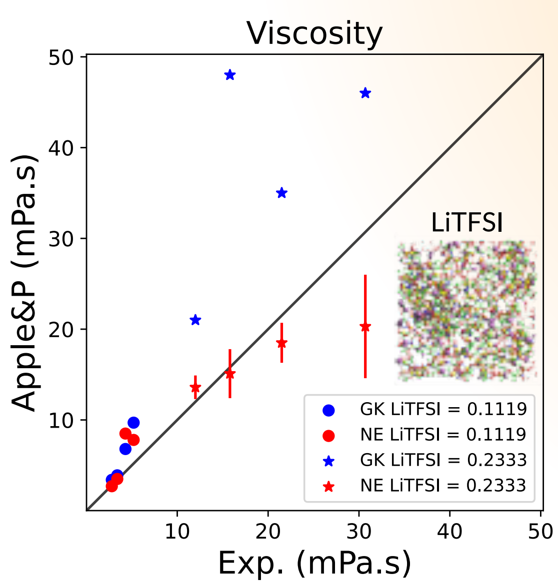
Key properties for battery R&D

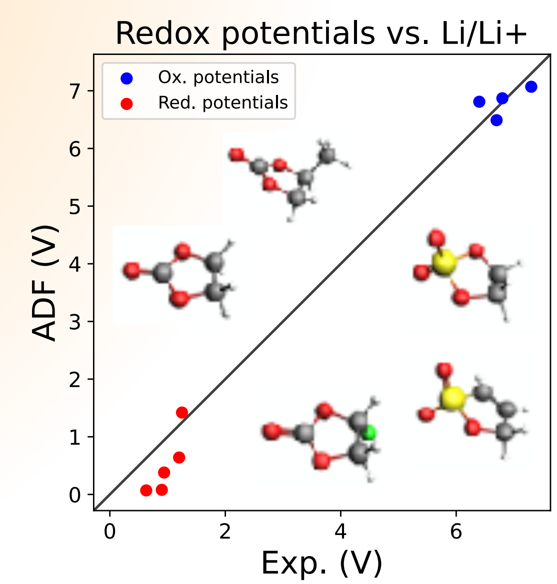
Connecting atomistic to experimental properties











- ✓ Energy density: intercalation potentials, voltage profiles
- ✓ Kinetics: diffusion coefficients, activation energy
- ✓ Thermodynamics & stability: free energy path, redox potentials, viscosity

➡ Require good model potentials

SCM Software for Chemistry & Materials

Summary

Next-Gen Battery Design: Harnessing the Power of AMS and ML

- The Amsterdam Modeling Suite
- Atomistic Modeling of Batteries
- Machine Learning Potentials in AMS
- Training Machine Learning Potentials with ParAMS
- MD Active Learning

The Amsterdam Modeling Suite

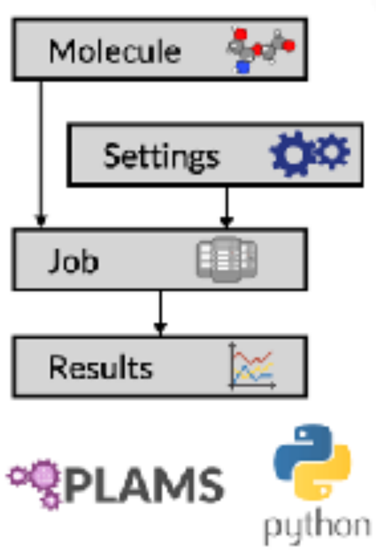
Comprehensive, user-friendly computational chemistry platform

Easy to deploy, switch between methods

- **Central AMS driver + computational engines**
  (Beyond) DFT, DFTB, ReaxFF, ML potentials
  Explore the potential energy surface
  Kinetics, Continuum Thermodynamics

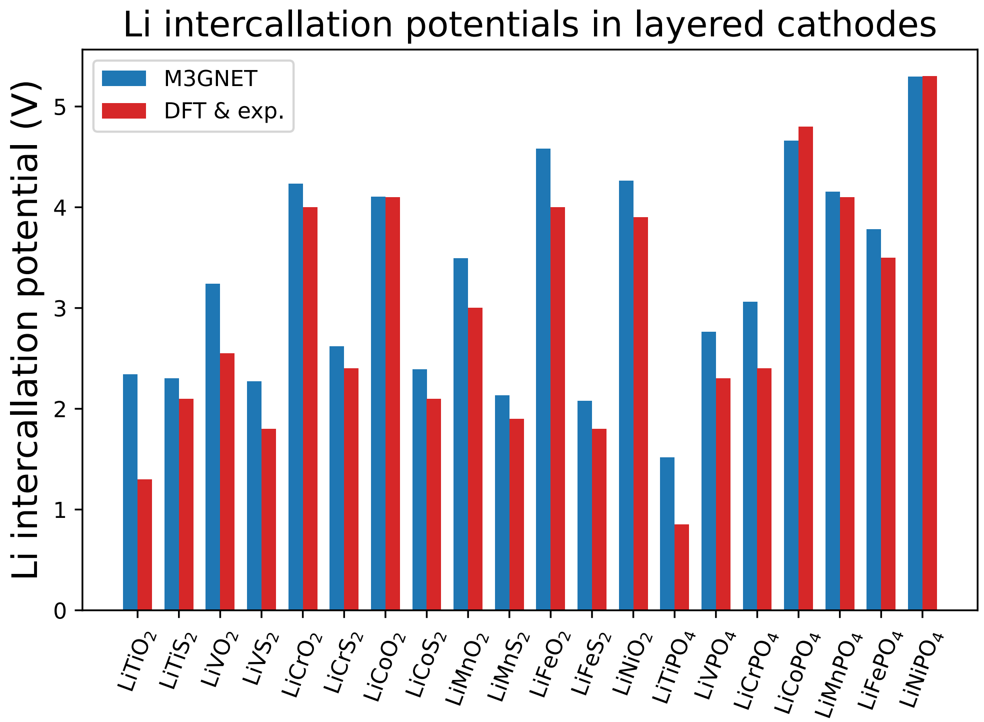
- **Graphical User Interface**
  Set up, visualize, analyze, run cross-platform

- **Python scripting environment**
  Powerful workflows
  Parametrization

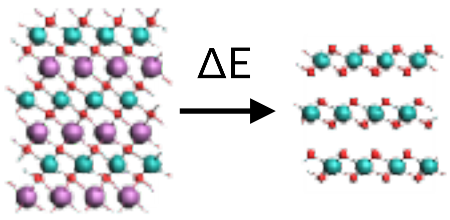


Batteries: energy density

Intercalation potentials & voltage profiles

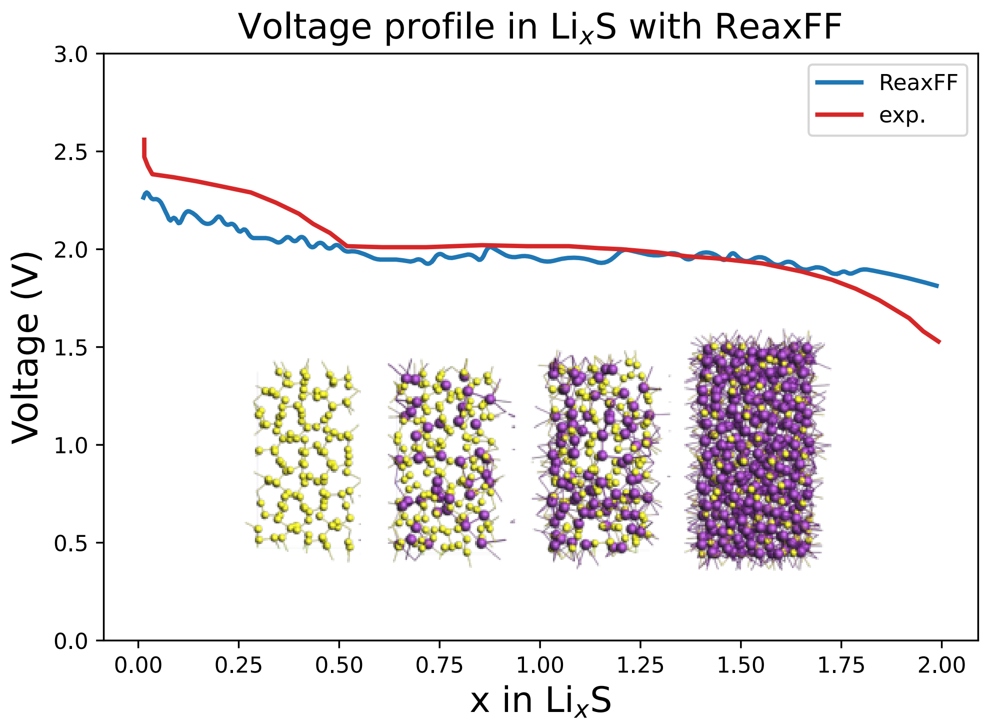


- Li intercalation potentials can be accurately predicted with DFT (limited to 100s atoms)
- M3GNet reproduces DFT with high accuracy
  - Li potential
  - Mechanical properties of the electrode (volume change upon lithiation)



Li_xCoO_2

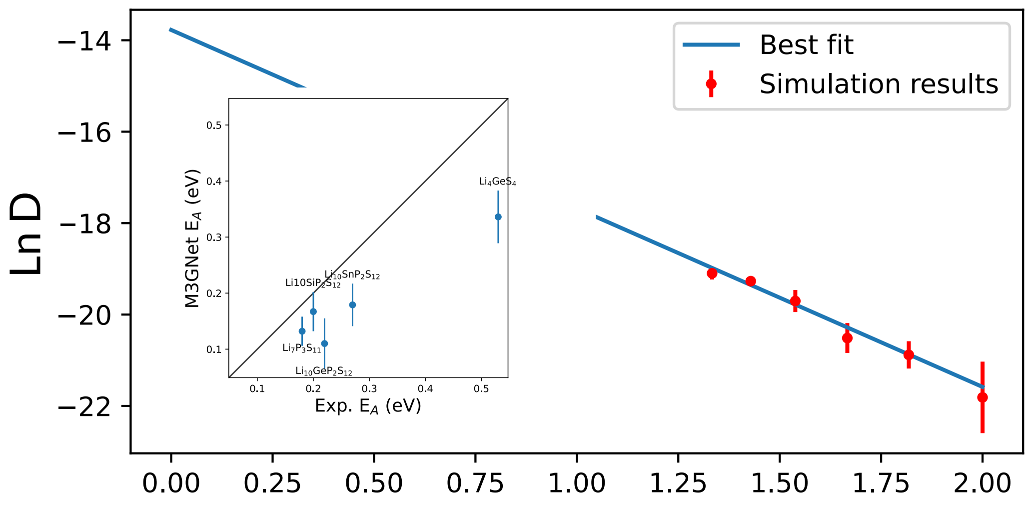
- Full lithium voltage profile
- Model amorphous electrodes
  - Use Grand-canonical Monte Carlo to model Li insertion
  - Evaluate volume change upon lithiation



Batteries: kinetics

Diffusion coefficients, activation energy

D300: 2.32e-12 +/- 4.59e-12 m² s⁻¹. Barrier: 0.336 +/- 0.047 eV

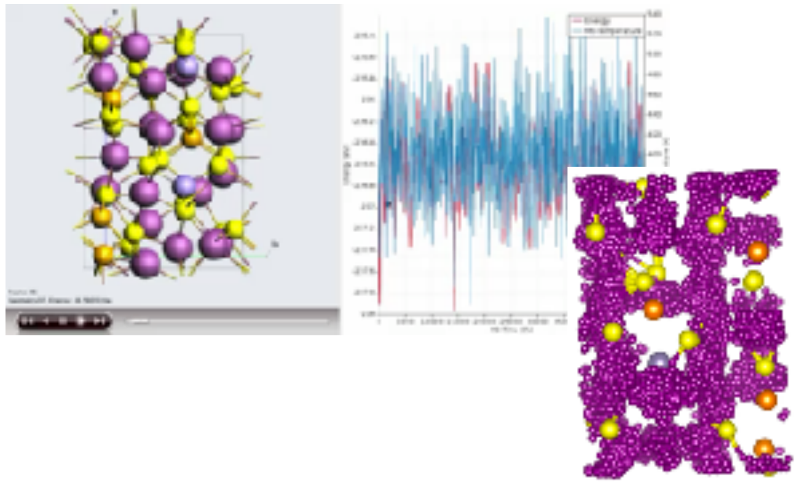


1000/T (K-1)

All in eV	EA	dEA	exp.
$Li_{10}GeP_2S_{12}$	0.110	0.045	0.22
$Li_{10}SiP_2S_{12}$	0.167	0.035	0.20
$Li_{10}SnP_2S_{12}$	0.179	0.038	0.27
Li_4GeS_4	0.336	0.047	0.53
$Li_7P_3S_{11}$	0.132	0.026	0.18

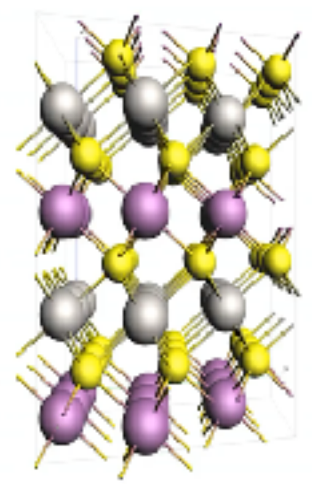
- Li diffusion from MD
  - Diffusion coefficients
  - Li diffusion path
  - Activation energy via Arrhenius

Superionic conductors $Li_{10}GeP_2S_{12}$

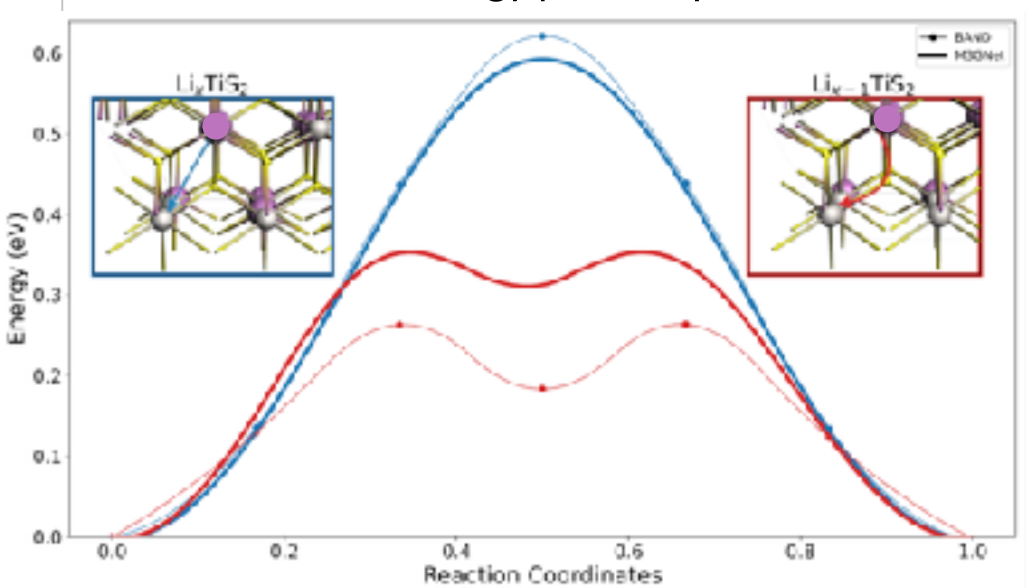


Crystals and exp. from Wang, Yan, et al. Nature materials 14.10 (2015): 1026-1031

- Li diffusion can be calculated with DFT based on NEB or PES scan
- MLP can accelerate the search by orders of magnitudes
  - Activation energy
  - Diffusion (kinetics)



Li minimum energy path in spinel $LiTiS_2$



Machine Learning Potentials

For accurate large-scale simulations

MLP

Pre-parametrized (or custom) models

- ✓ ANI-1ccx & ANI 1x (H, C, O, N)
- ✓ ANI-2x (H, C, O, N, F, S, Cl)
- ✓ AIMNet2 (H, B, C, N, O, F, Si, P, S, Cl, As, Se, Br, I) + PBC
- ✓ M3GNet (Universal)

ParAMS
Train M3GNet
AIMNet2

Active Learning

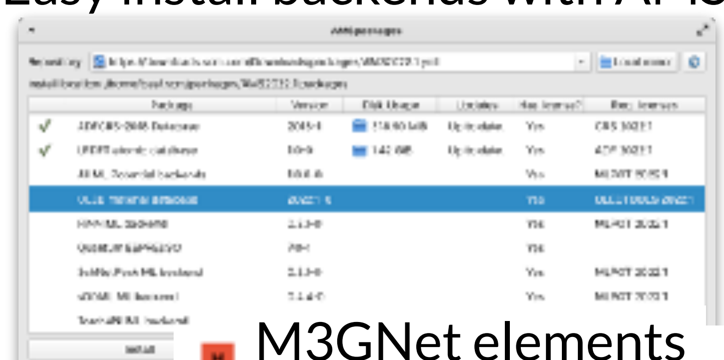
AMS driver

ASE

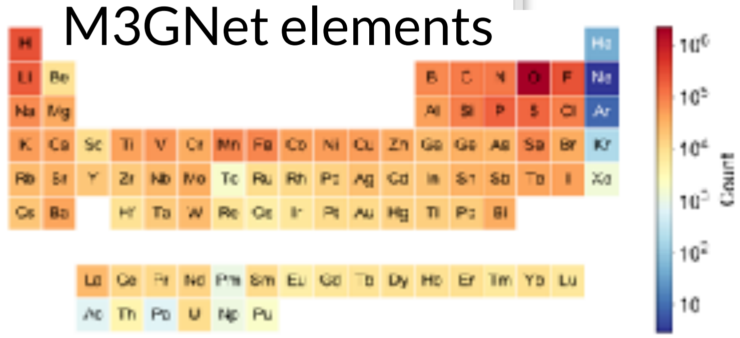
Any model ASE-compatible

- ✓ ALIGNN-FF
- ✓ CHGNet
- ✓ DeepMD-kit
- ✓ Open Catalyst Project
- ✓ etc.

Easy install backends with AMSpackages



M3GNet elements



CUDA-enabled PyTorch and Tensorflow

Use MLP with any tasks of the AMS driver

Tasks

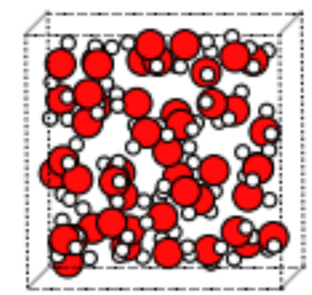
- Molecular dynamics
- Frequencies & phonons
- Stress & elastic tensors
- Scan coordinates & constraints
- Monte Carlo & GCMC, etc.

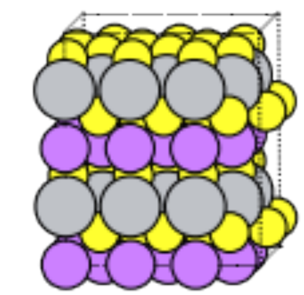
- *O. Isayev et al. Chem. Sci., 8, 3192–3203, 2017*
- *Shyue Ping Ong et al. Nature Computational Science 2, 718–728, 2022*
- *Simon Batzner et al. Nature Communications volume 13, 2453, 2022*
  S. Chmiela et al. Comp. Phys. Commun. 240, 38-45, 2019
- *K. T. Schütt et al., J. Chem. Theory Comput. 15, 448-455, 2019*
- *Deng, Bowen, et al. Nature Machine Intelligence 5.9, 1031-1041, 2023*
- *Choudhary, Kamal, and Brian DeCost. npj Computational Materials 7.1, 185, 2021*
- *Zhang, Linfeng, et al. Physical review letters 120.14, 143001, 2018*
- *Zitnick, C. Lawrence, et al. arXiv preprint arXiv:2010.09435, 2020*

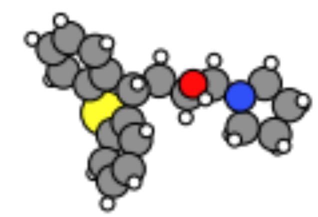
Pre-trained MLPotentials

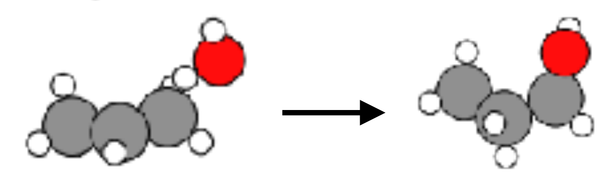
Examples where the universal potential M3GNet is inaccurate

System	Quantity	M3GNet-UP	Reference DFT	Exp.
Liquid water	Density (g/cm^3)	0.95	1.01	1.00
Liquid water	Self-diffusion (10^{-9} m^2/s)	0.23	2.6	2.3
$LiTiS_2$	Li migration E_A (eV)	0.39	0.86	
$C_{20}H_{23}NOS$	Conformers energy RMSE vs. DFT (eV)	2.01		
Propene + water	Reaction energy (eV)	1.65	2.75	









⚠️ Always test/validate pre-trained models toward your targeted application

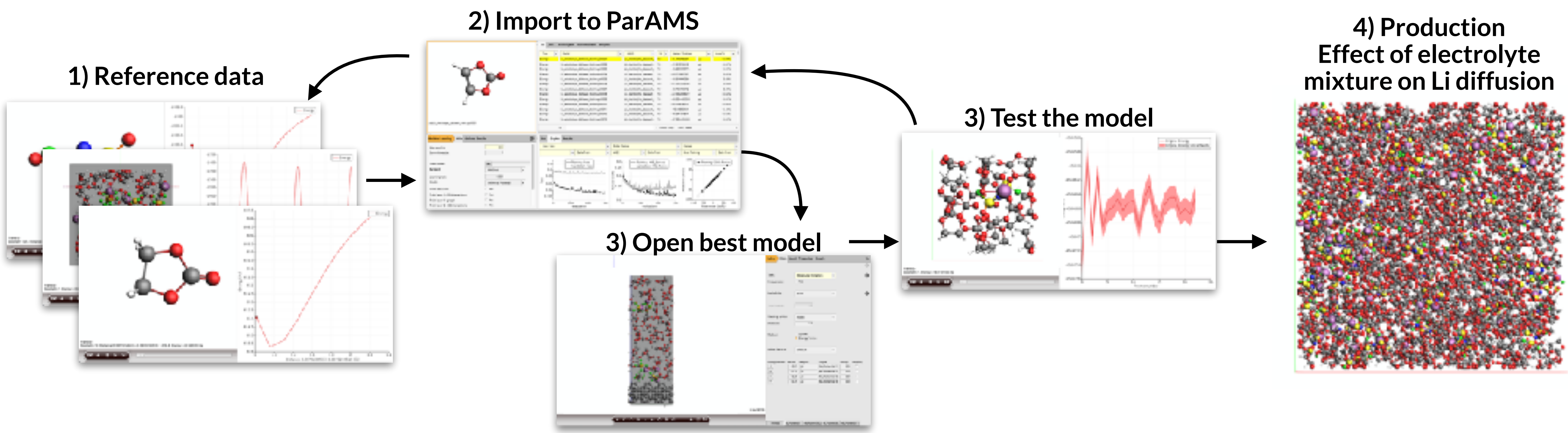
What to do if the pre-trained model is not accurate enough?

➡ Custom models

Custom models

Train M3GNet based on a dataset of reference calculations

1. Prepare a dataset of reference calculations
   Volume scans, MD, NEB, defects, etc.
2. Use **ParAMS** to manage data and to train M3GNet/nequip/AIMNet2
   Compatible with AMS, VASP, QE, Gaussian, etc.
   Split the dataset into training, validation, test
   Train M3GNet-like model, from scratch or fine-tune universal model
   Train committee models
3. Import optimized model in AMSinput
   Test the new optimized model
4. Production



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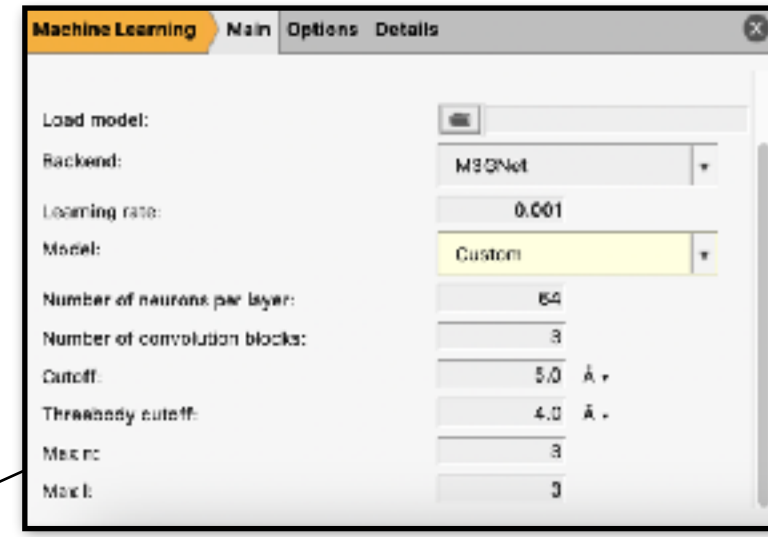

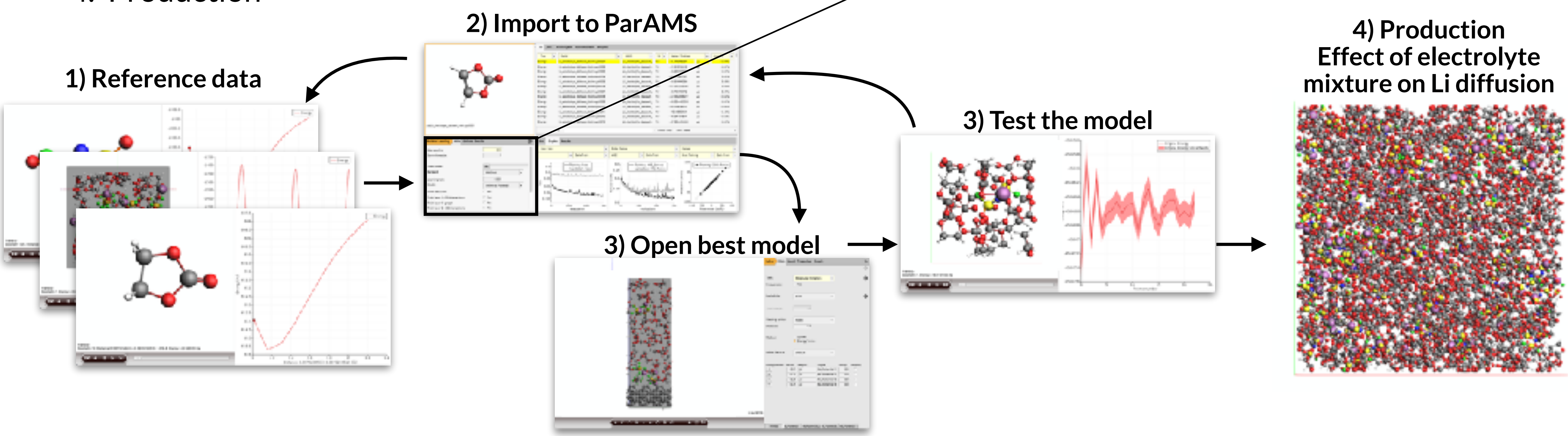

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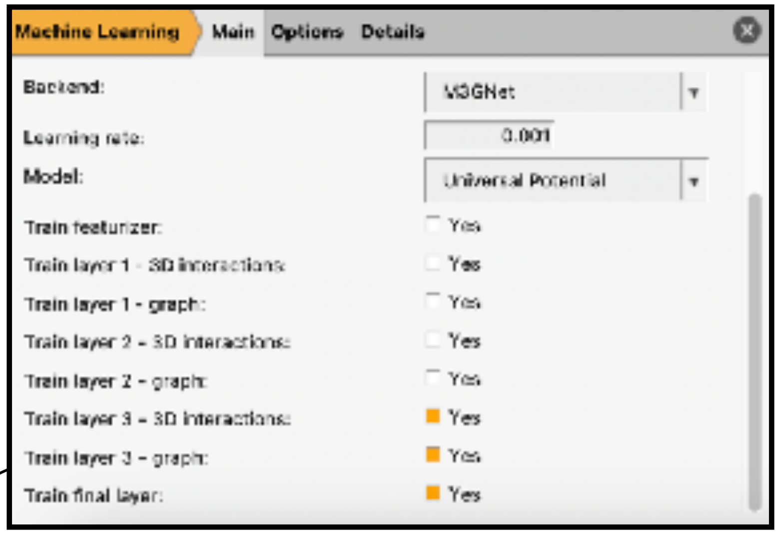

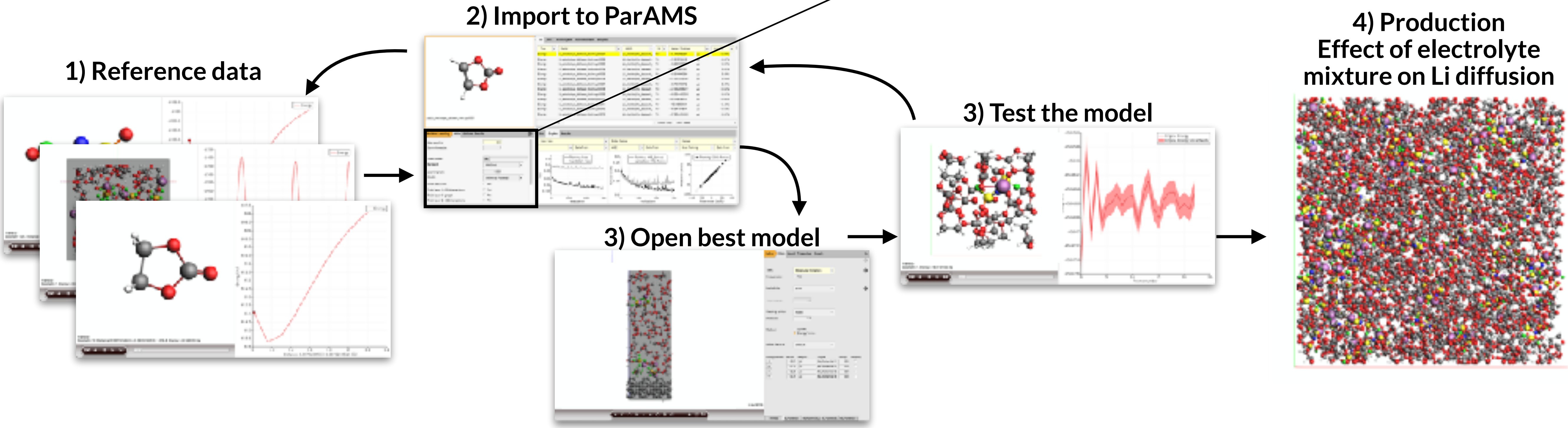

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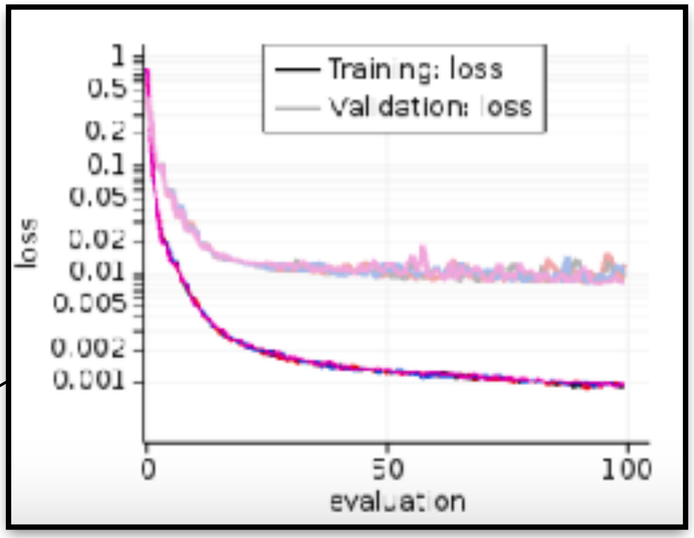

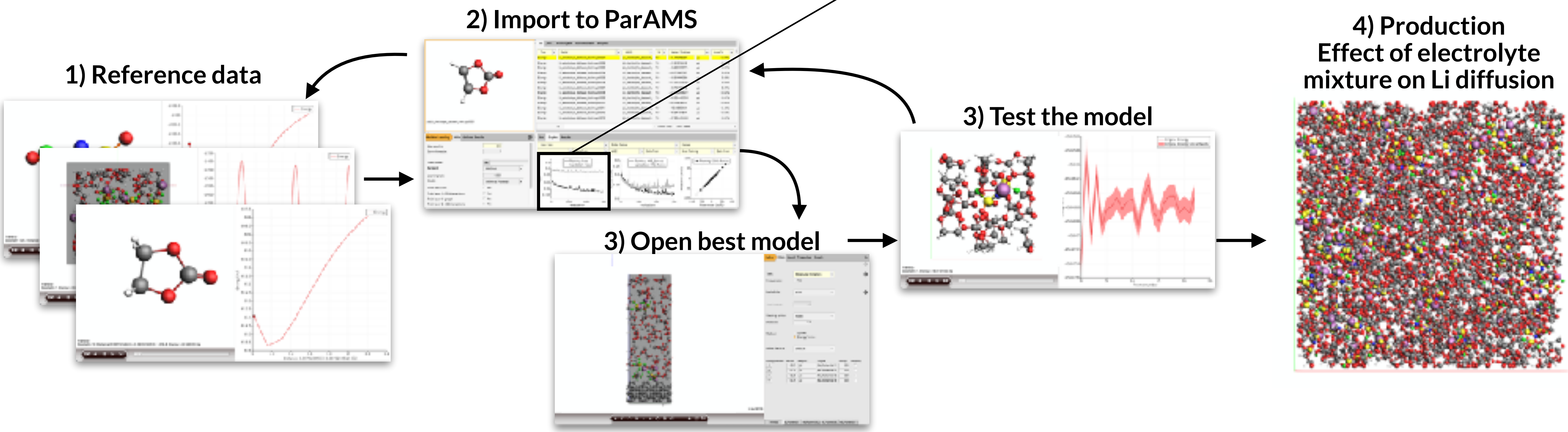

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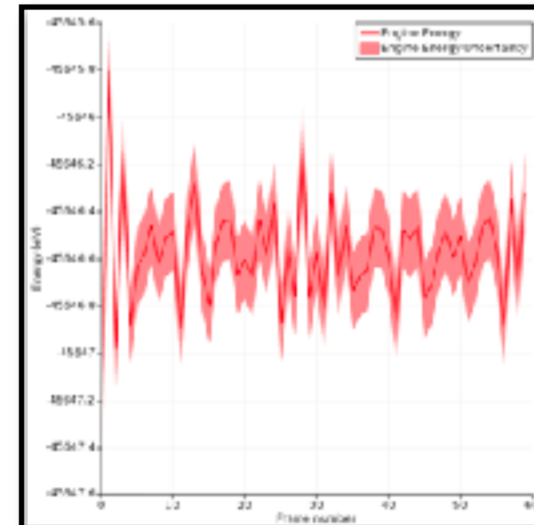
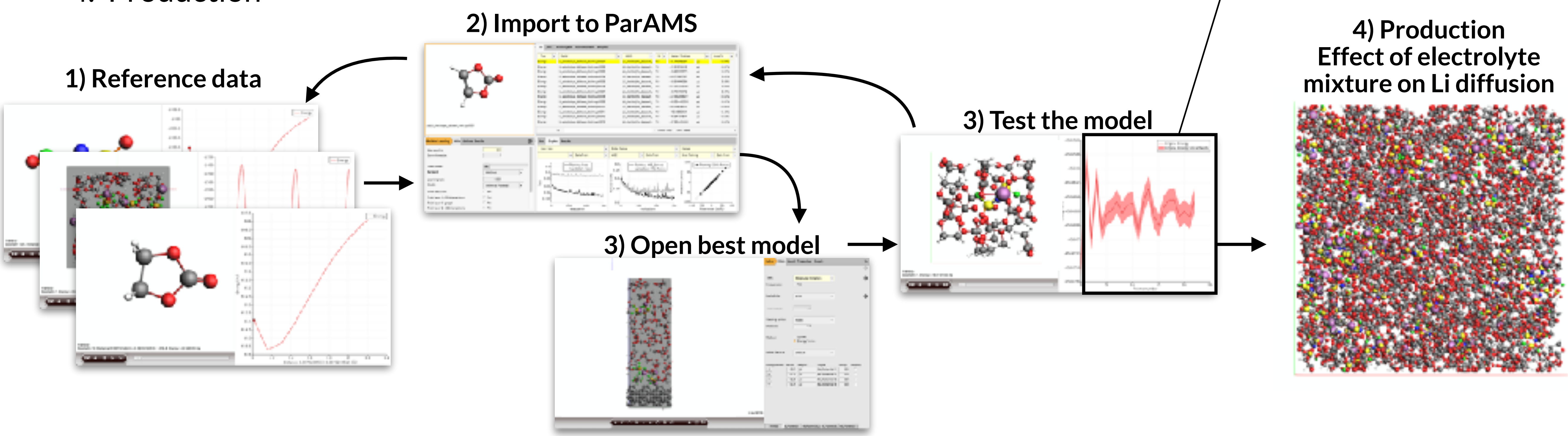


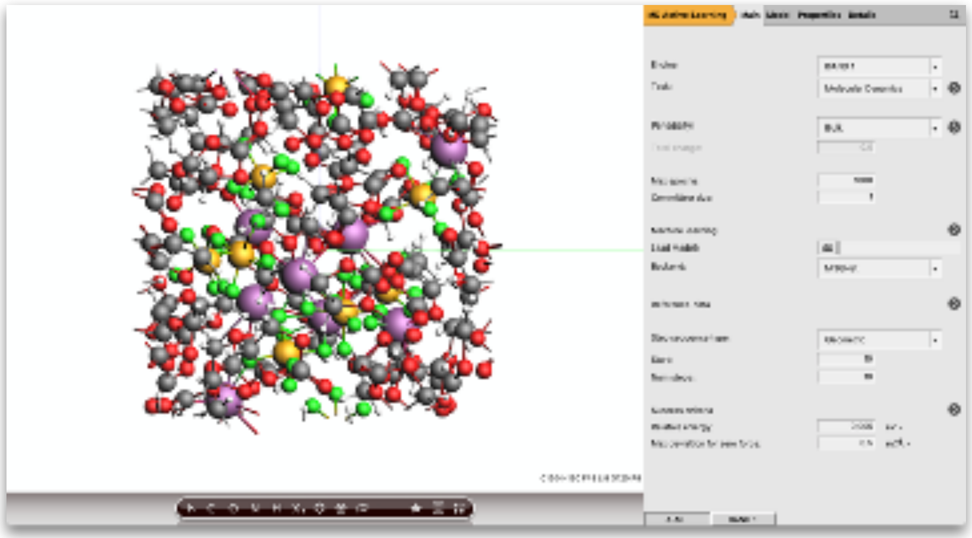


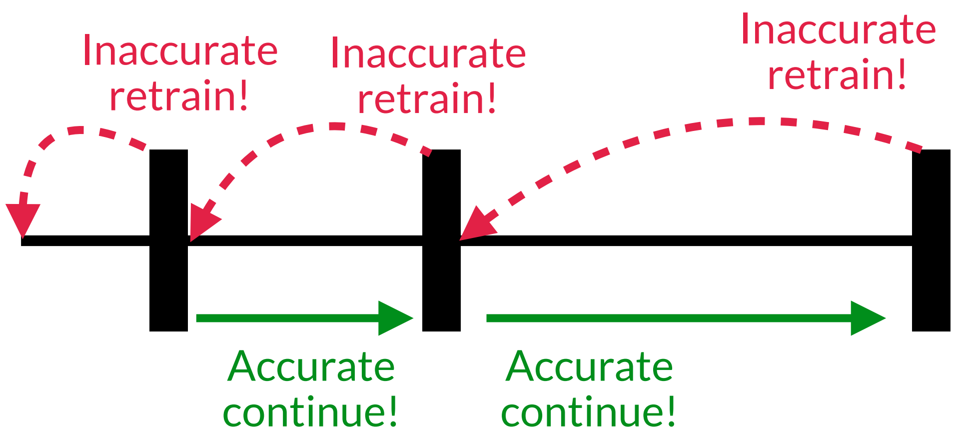
Custom models

Active learning MD: workflow

- Ingredients
  - Reference engine: AMS-QE / PBE-D3
  - Task(s): MD, NEMD
  - ML model: M3GNet, architecture, fine-tune
  - Parameter optimization: **ParAMS**
- Recipe
  - Reaction boost, reactor, etc.
  - If geometry inaccurate, launch DFT, retrain
  - Continue MD, loop

GUI support



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   2        2  SUCCESS  Accurate                                  0.2650
   3        1  FAILED   Inaccurate                                0.5041
   3        2  FAILED   Inaccurate                                0.3247
   3        3  SUCCESS  Accurate                                  0.1949
   4        1  FAILED   Inaccurate                                0.6299
   4        2  SUCCESS  Accurate                                  0.2259
   5        1  FAILED   Inaccurate                                0.3347
   5        2  SUCCESS  Accurate                                  0.1636
   6        1  SUCCESS  Accurate                                  0.2210
   7        1  FAILED   Inaccurate                                0.3427
   7        2  SUCCESS  Accurate                                  0.2000
   8        1  SUCCESS  Accurate                                  0.2614
   9        1  FAILED   Inaccurate                                0.1858
   9        2  SUCCESS  Accurate                                  0.1190
  10        1  FAILED   Inaccurate                                0.3466
  10        2  SUCCESS  Accurate                                  0.1212
  11        1  SUCCESS  Accurate                                  0.2718
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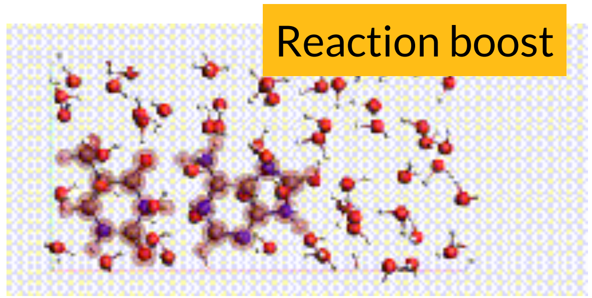

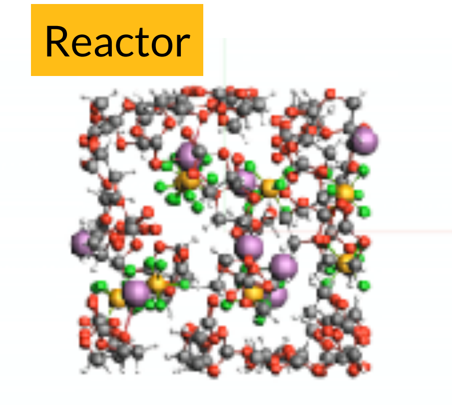

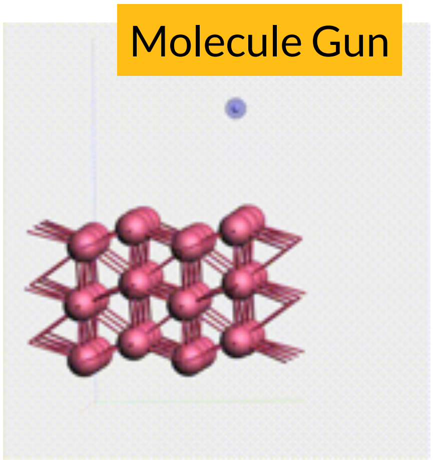

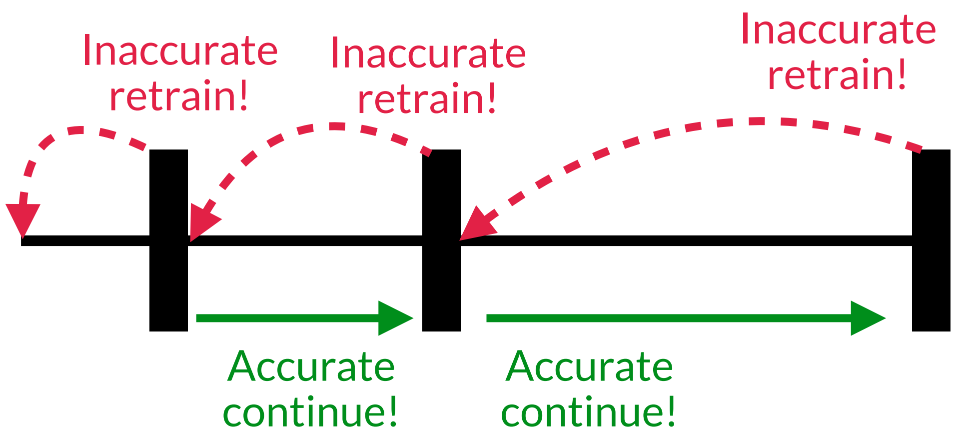


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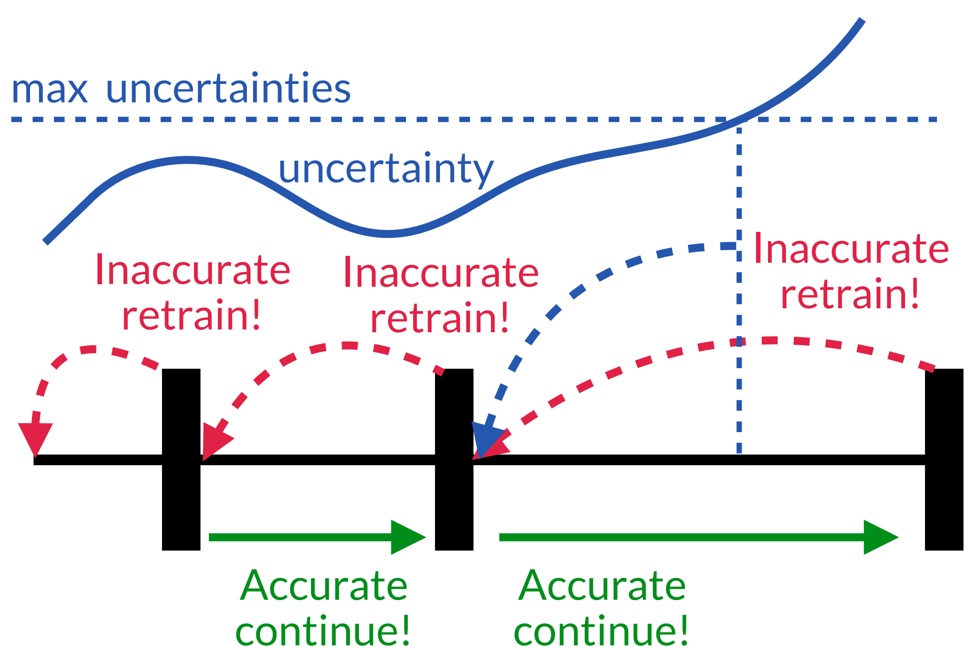


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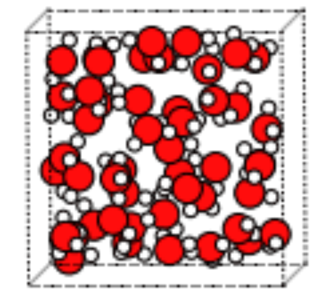
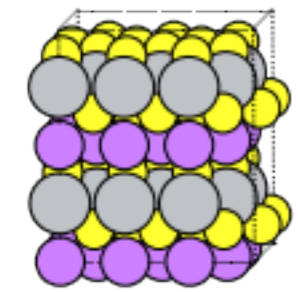
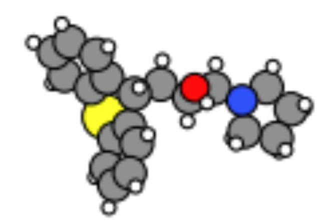
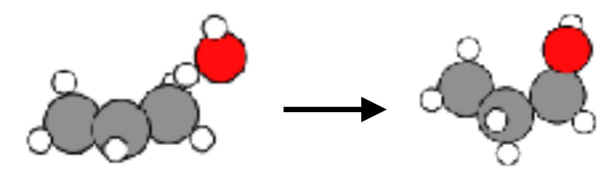
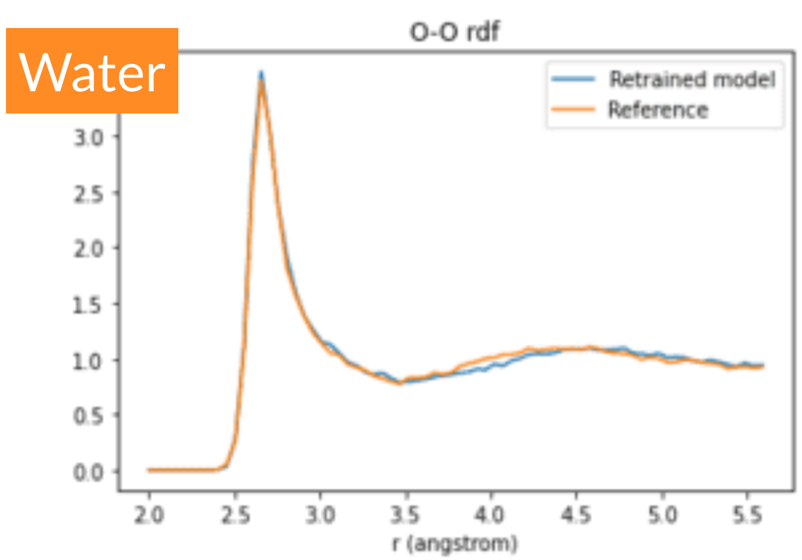
--- End summary ---
```

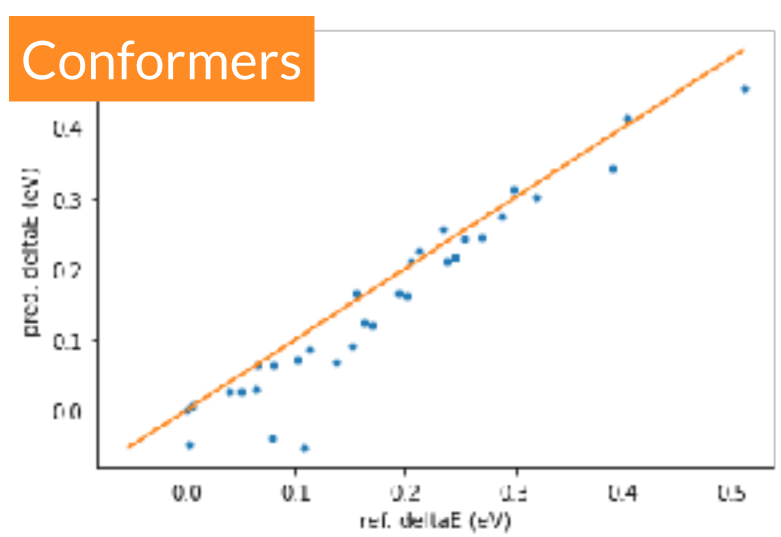
Custom models

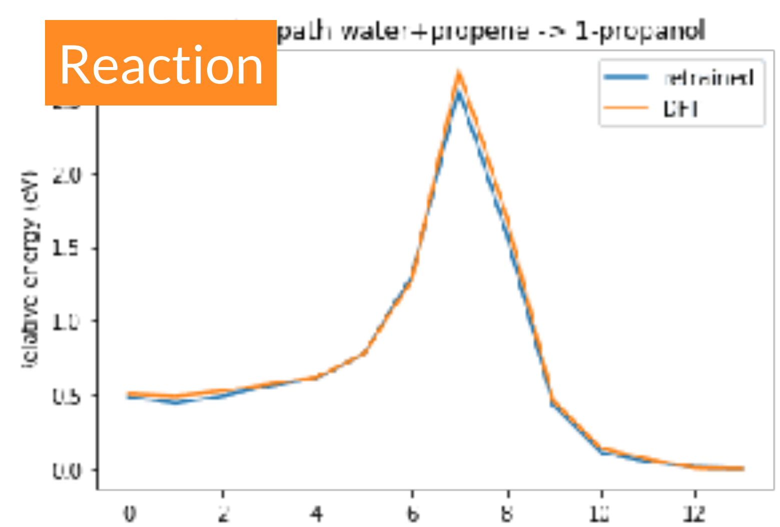
Active learning MD: results

System	Quantity	M3GNet-UP	M3GNet-custom	Reference DFT	Exp.
Liquid water	Density (g/cm^3)	0.95	1.02	1.01	1.00
Liquid water	Self-diffusion (10^{-9} m^2/s)	0.23	2.5	2.6	2.3
$LiTiS_2$	Li migration E_A (eV)	0.39	0.8	0.86	
$C_{20}H_{23}NOS$	Conformers energy RMSE vs. DFT (eV)	2.01	0.40		
Propene + water	Reaction energy (eV)	1.65	2.55	2.75	



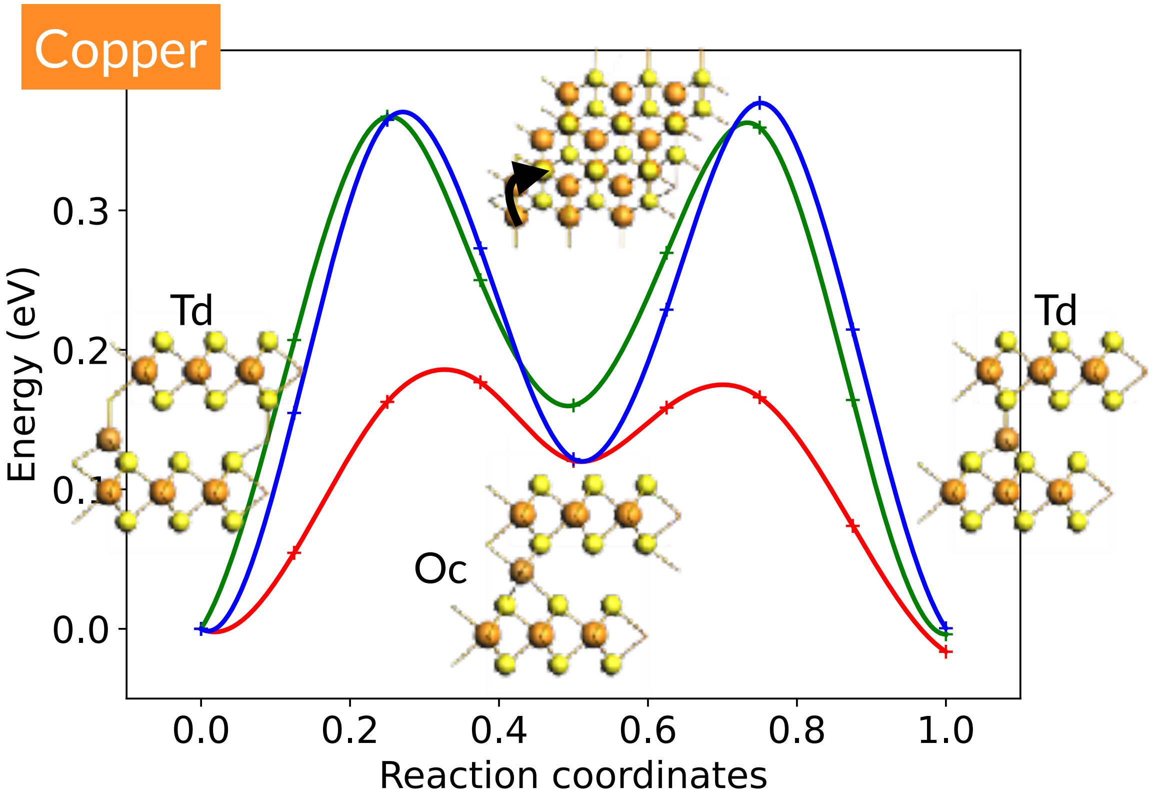


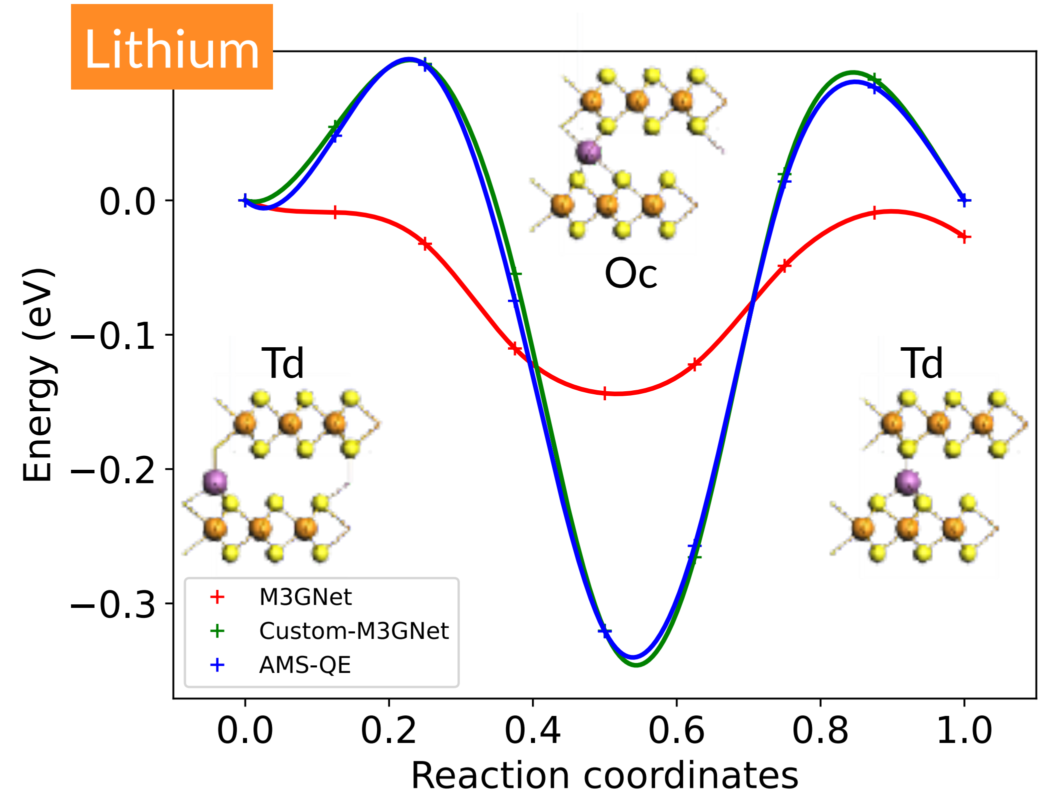


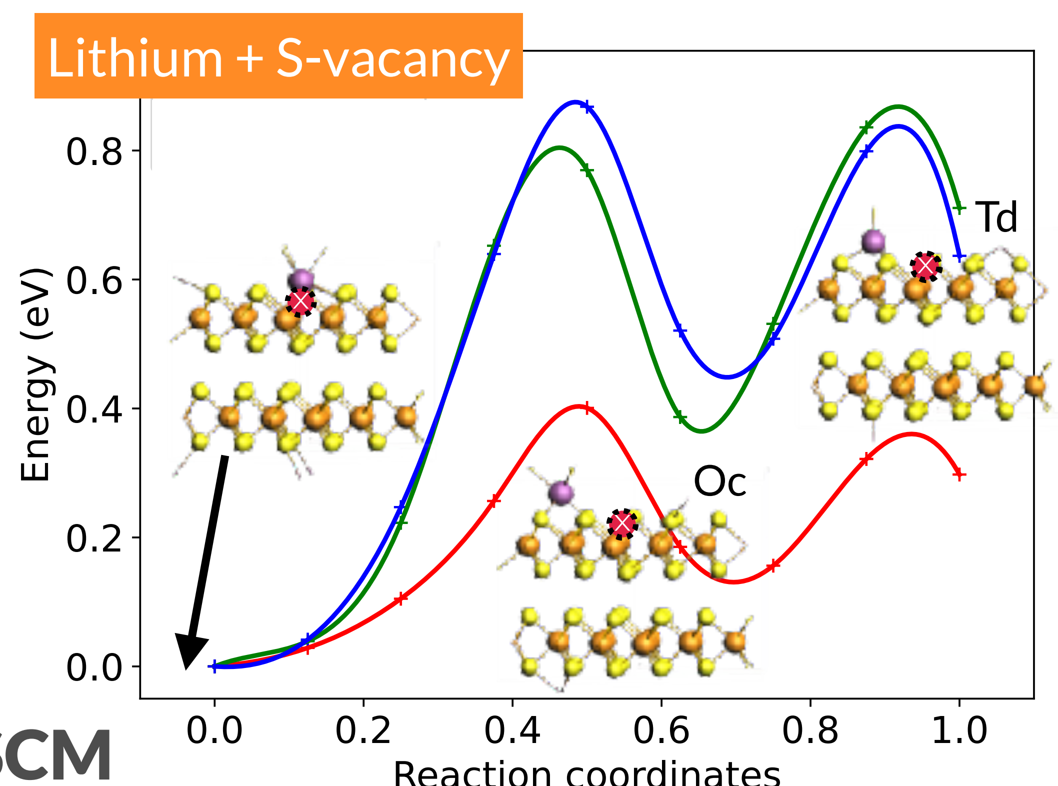
https://www.scm.com/doc/Workflows/SimpleActiveLearning/PythonExamples/PythonExamples.html

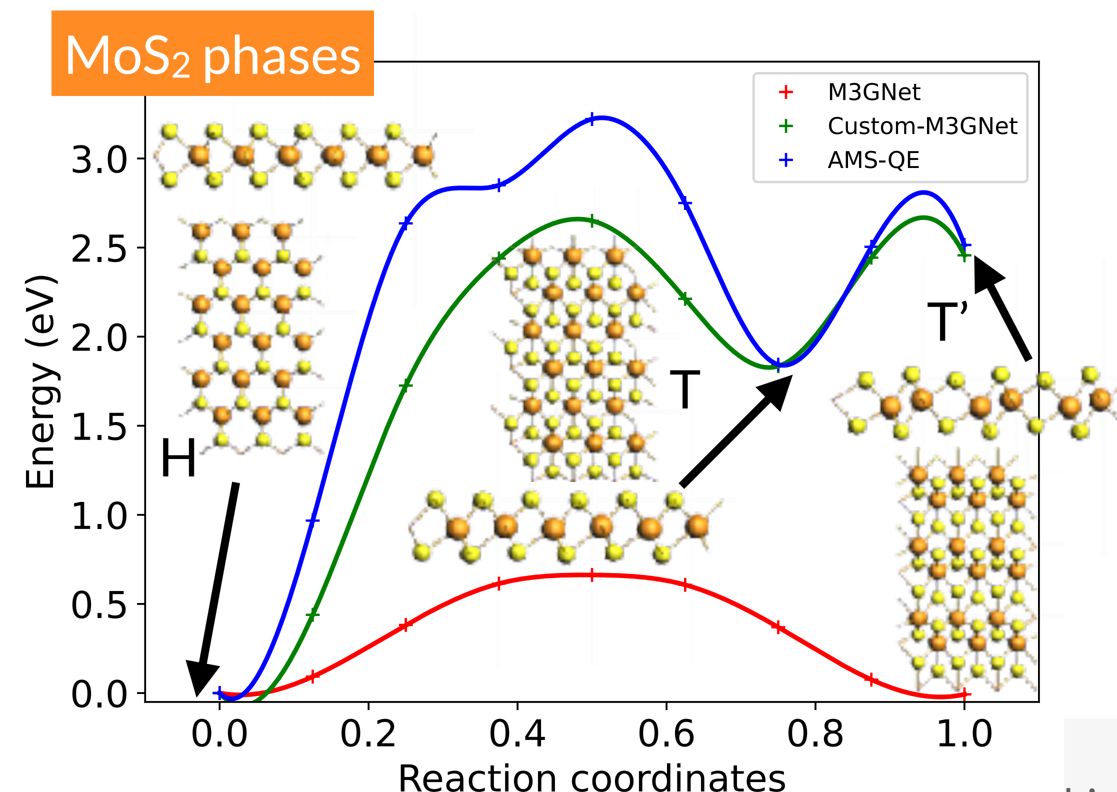
Custom models

Active learning MD: results









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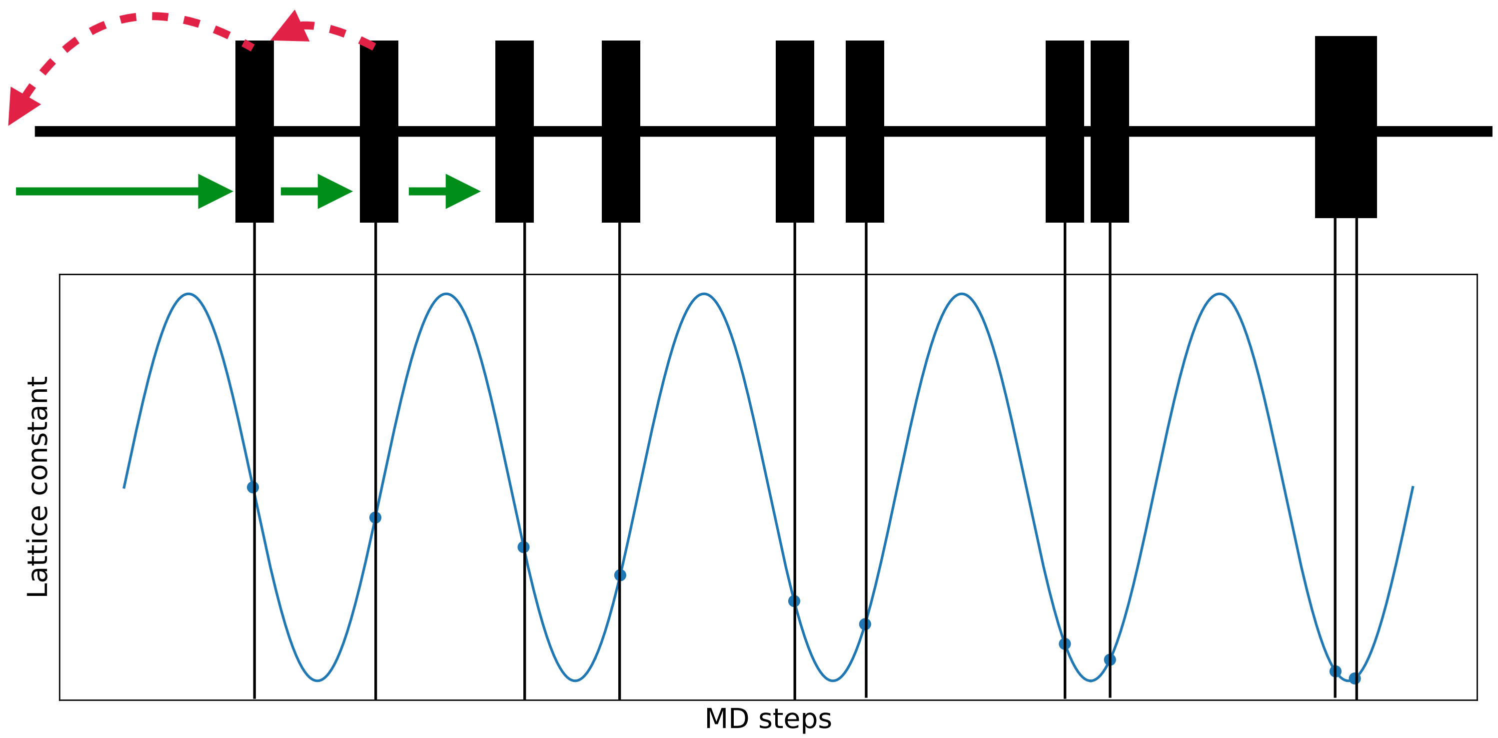
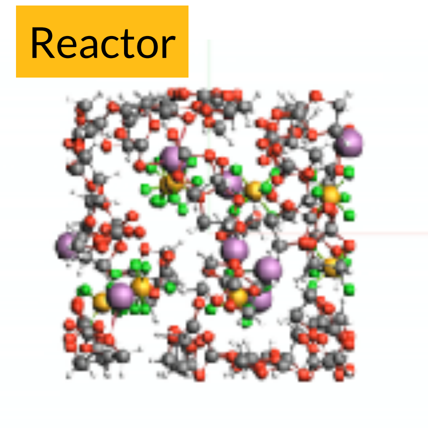
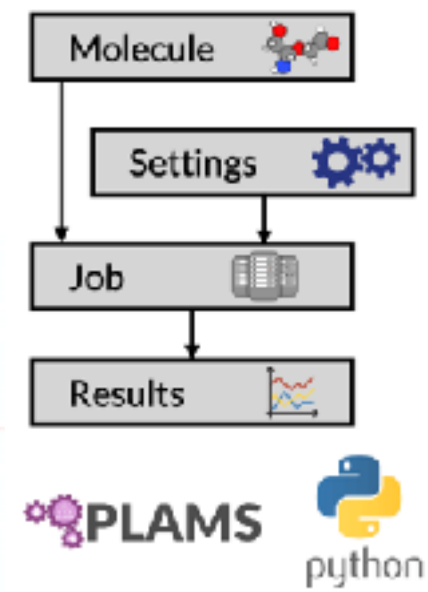
Software for Chemistry & Materials

Custom models

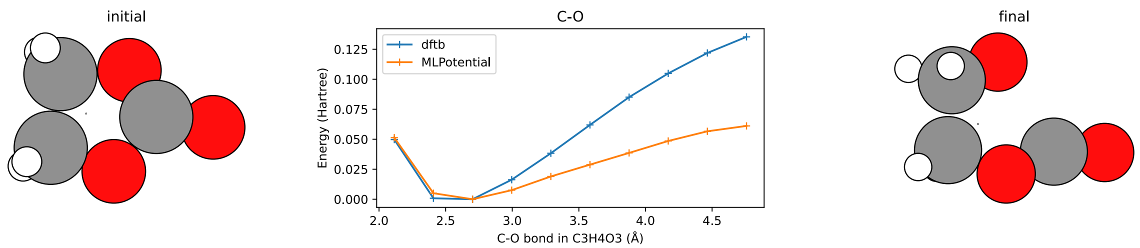
From active learning to complex workflows

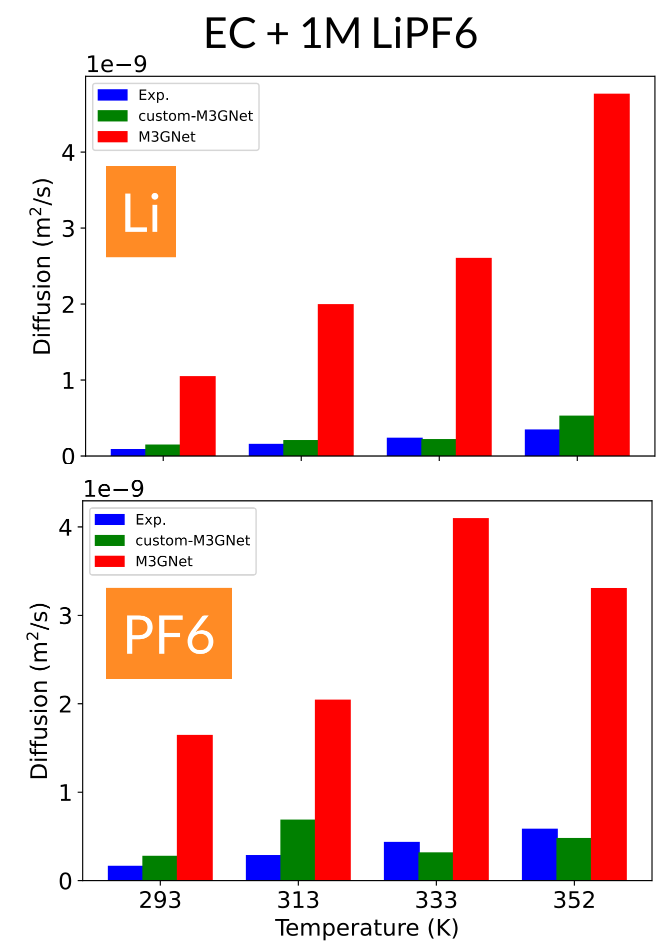






- Training: initial dataset / ParAMS training, **multiple AL in series**
- Toward reactive MLPot: identify molecules, reactions to **augment the dataset**
- Production: workflow scan density, NPT, NVT, etc.





The SCM team

Making Computational Chemistry Works for You!

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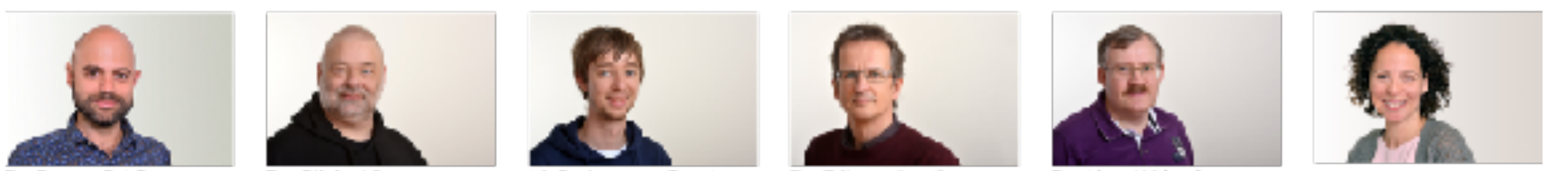

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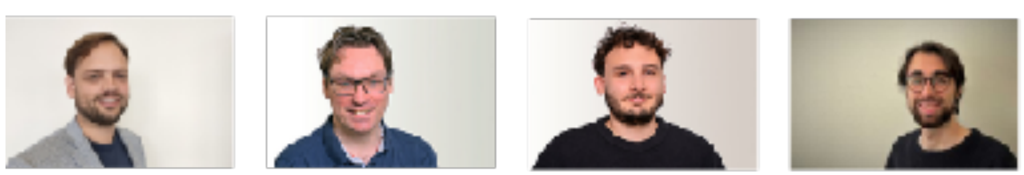

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Thank you for your attention!

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