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Machine Learning and Molecular Dynamics:

MedeA Machine-Learned Potential (MLP) and Machine-Learned Potential Generator (MLPG) Modules

David Reith
Materials Design

Nov 2, 2021

Materials Design UGM

UGM 2021

The Materials Design annual user event will be online again for 2021.

Plenary Speakers include:

Prof. Michele Parrinello
Prof. Georg Kresse
Prof. Richard Catlow

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Email

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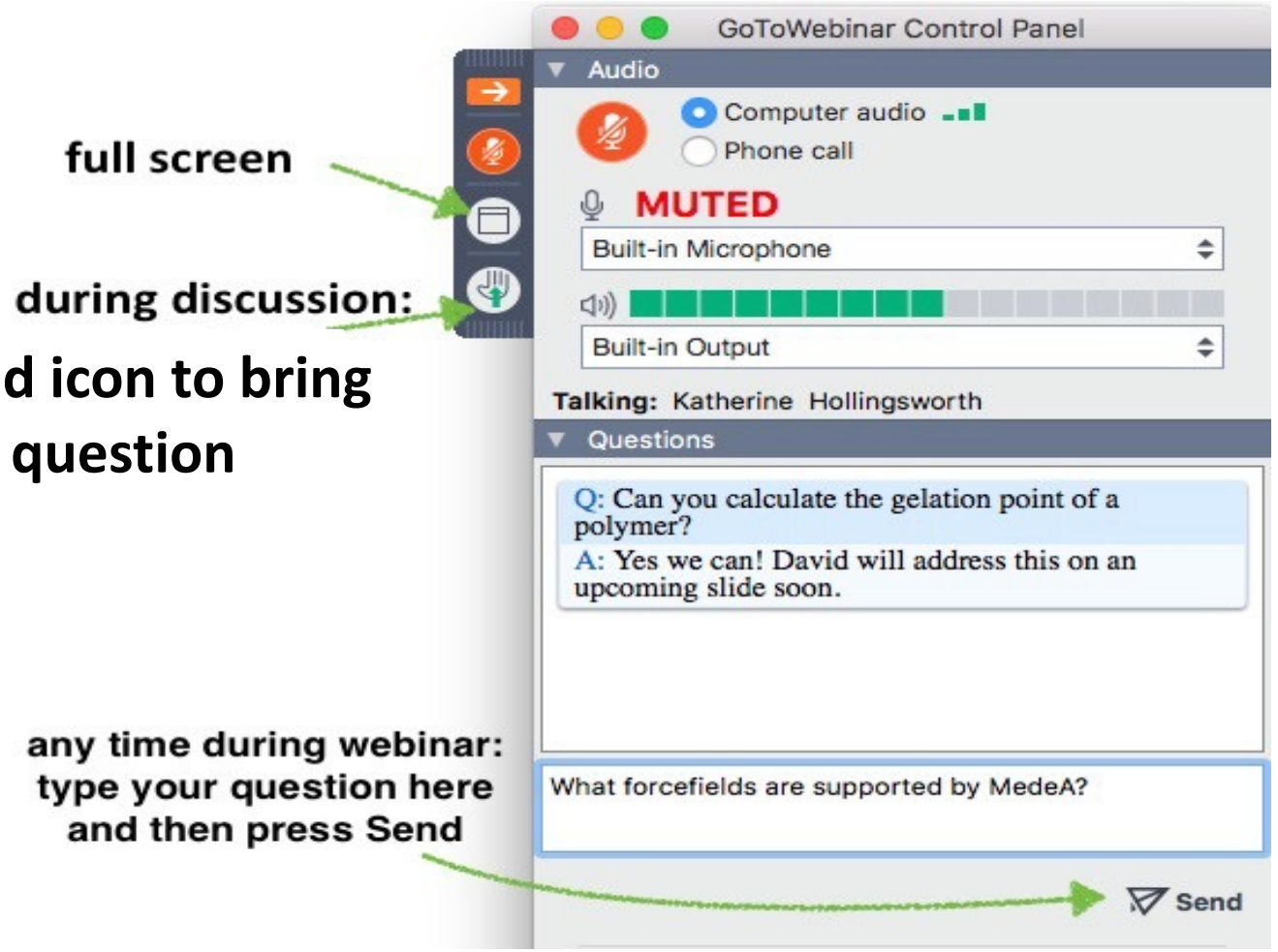
Materials Design UGM Training Sessions

- Tuesdays in this UGM series will feature online training sessions with members of the Materials Design Team
- Share the training sessions with your colleagues!
  - Registration details
    - https://ugm.materialsdesign.com
- We will be recording this session
  - Upcoming sessions are posted on the UGM site
  - Watch any of our earlier webinars anytime www.materialsdesign.com/webinars
- Audio issues
  - Log out and log back in again
  - Check your audio output
  - Google Chrome (most recent 2 versions) Mozilla Firefox (most recent 2 versions) Apple Safari (most recent 2 versions) Microsoft Edge (most recent 2 versions)

Please Ask Questions!



Use the raise hand icon to bring attention to your question

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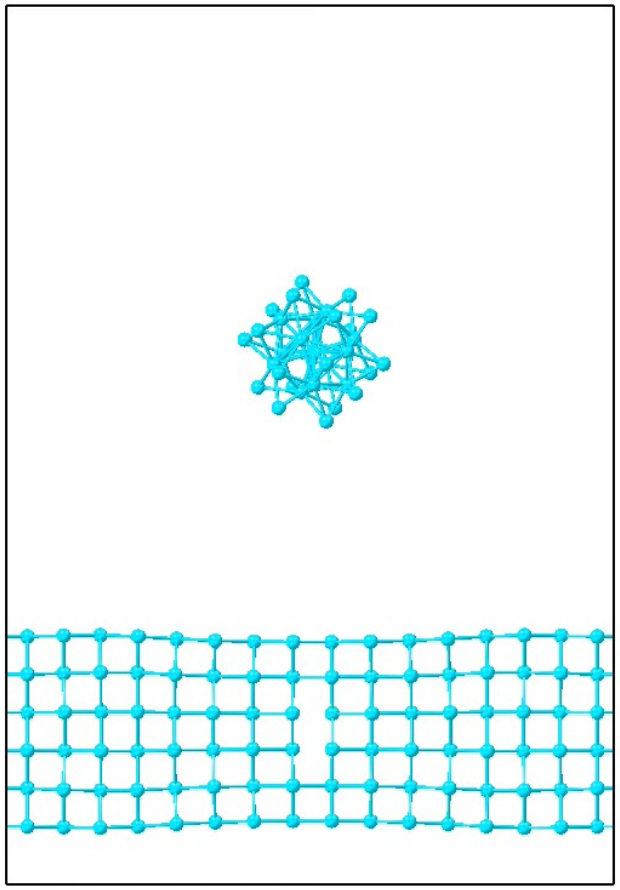

Niobium nanocluster impacts a 110 Nb surface with a velocity of 20 Å/ps
(2 km/s or 7200 km/h ~ 0.84 moon escape velocity)

802 Nb atoms
5 ps equilibration and 10 ps simulation

Outline

- Overview and introduction to machine-learned potentials
- Building a machine-learned potential to simulate the impact of niobium clusters on a niobium surface
- Extend the machine-learned potential to include oxygen to study oxygen desorption
- Build a water machine-learned potential
- General MLP guidelines and conclusion

Overview of Materials Simulation Methods

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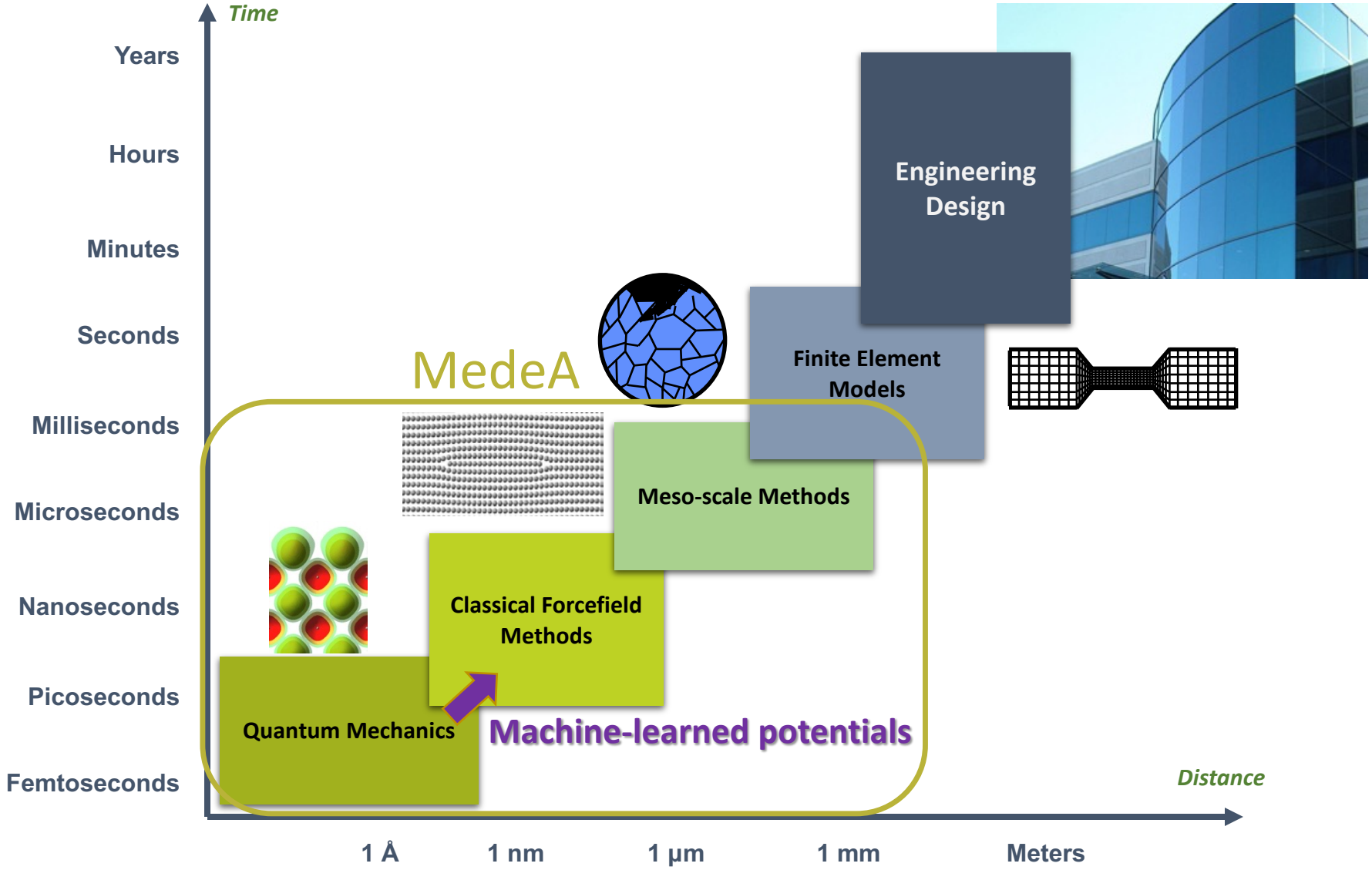

Machine-Learned Potentials

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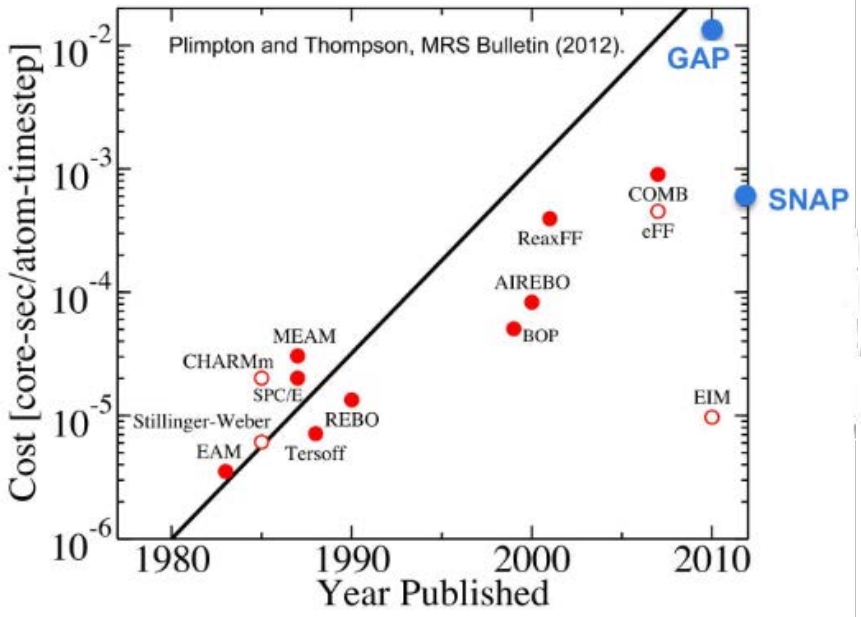
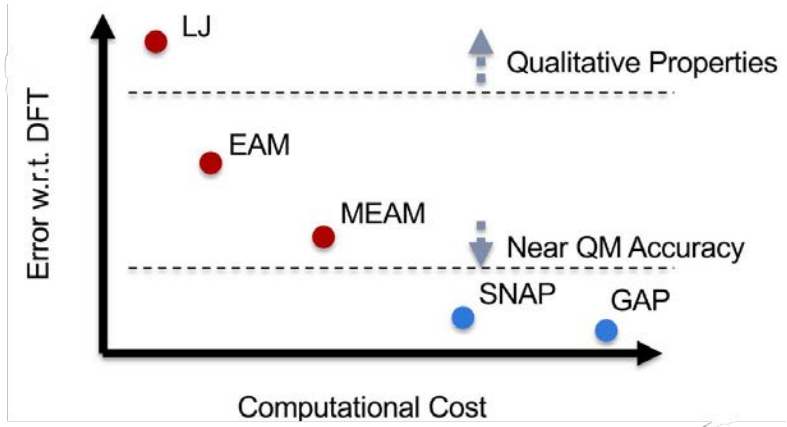
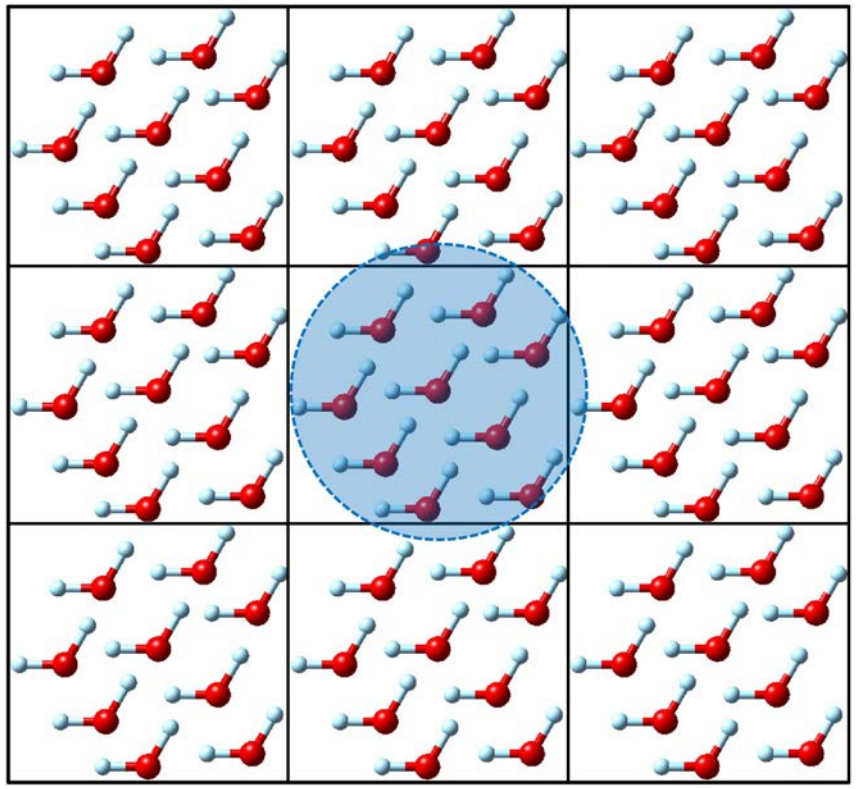
- Bridging the time and length scale with VASP accuracy at LAMMPS speed
- Build a tailor-made potential for your research
- Reactive by construction
- Generation of a MLP almost automatic from a training set
- Spectral Neighbor Analysis Potentials (SNAP*)
  - Kernel based method
  - MedeA uses FitSNAP to create SNAP potentials





* A.P. Thompson *et al.,* J. Comput. Phys. **285**, 316-330 (2015)

Machine-Learned Potentials



- Partition structures into local atomic environments
- Local atomic structures described in terms of relative atom positions and types

$$B_i = B_i\left(\{\boldsymbol{r}_{ji}, A_j, j = 1, N_i\}\right),\ i = 1, N$$

  - $\boldsymbol{r}_{ji}$ in local coordinates (r, ϑ, φ), or
  - all pairwise distances r_{jl} in cluster
  - N: all atoms, N_i: all atoms in sphere i

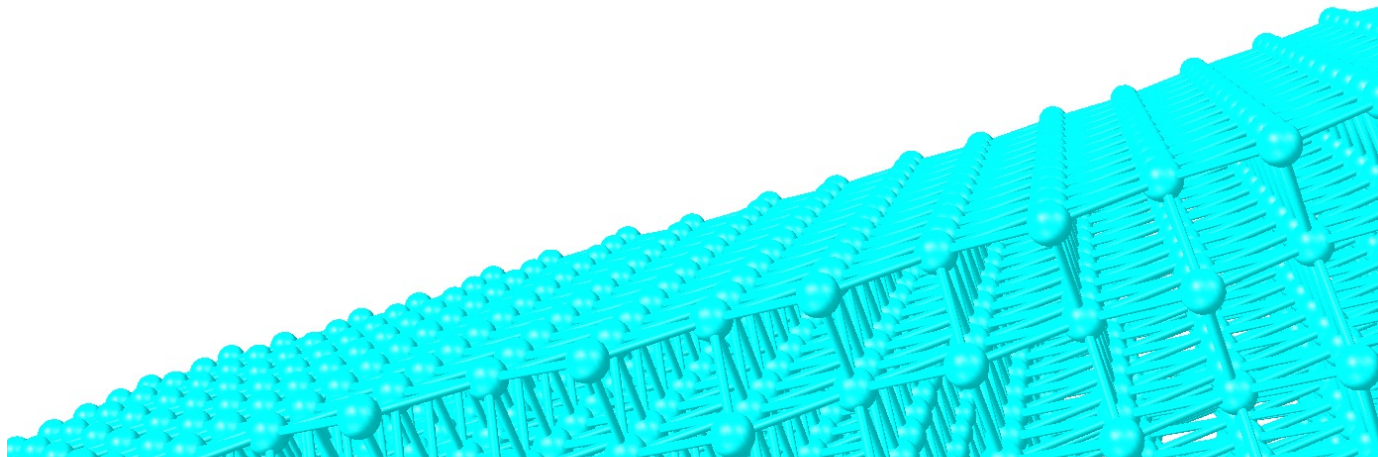
- Local energy centered at atom i

$$E_i = \beta_0 + \Sigma_k \beta_k B_{i,k}$$

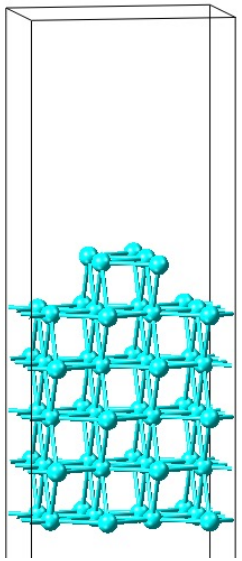
- Total energy

$$E = \Sigma_i E_i$$

Niobium Surface Machine-Learned Potential



Procedure

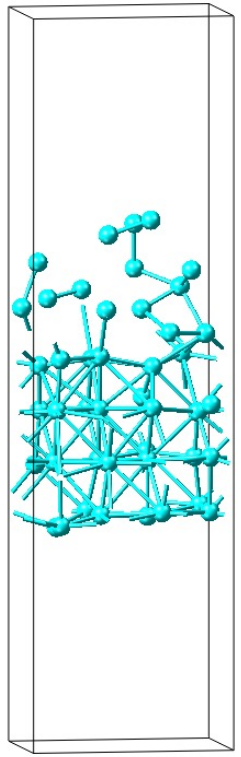


Build a (110) Nb surface slab with 44 atoms

- Start with **Nb.sci** in `C:\MD\Structures\Elements\`
- Build a h: 1, k: 1, l: 0 surface slab with 3 repeat units and a gap of 20 Ang.
- Create a 2x2x1 supercell
- Delete 2 Nb atom rows on one surface side

Use VASP to run an ab initio MD simulation for 400 fs on this model (time step 4 fs)

- **Calculation** tab
  Type of calculation: Molecular Dynamics, **Ensemble:** temperature scaling (nVE), **Simulation time:** 400 **fs**, **Temperature initial:** 300 **K**, **Temperature end:** 4000 **K**, **Planewave cutoff:** 350 **eV**, **Projection:** Real space
- **SCF** tab
  Spacing of k-points: 0.4 **1/Ang**, ☒ **Use odd size grids**, **Type of smearing:** Gaussian



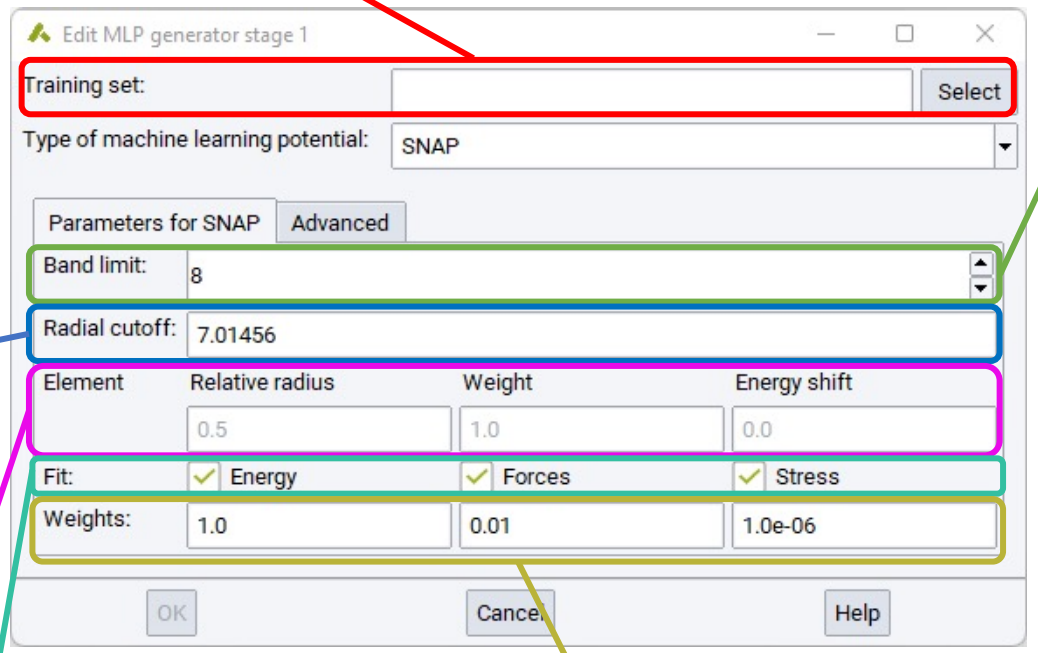
Use the MD trajectory to train a SNAP MLP

- **Parameters for SNAP** tab
  Band limit: 12
- **Advanced** tab
  Optimize ☒ **Radial cutoff** ☒ **Relative radii** ☒ **weights**

Apply the MLP to run a 15 ps MD simulation with LAMMPS for a surface slab with impacting Nb nano particle containing 802 atoms

Machine-Learned Potential Generator

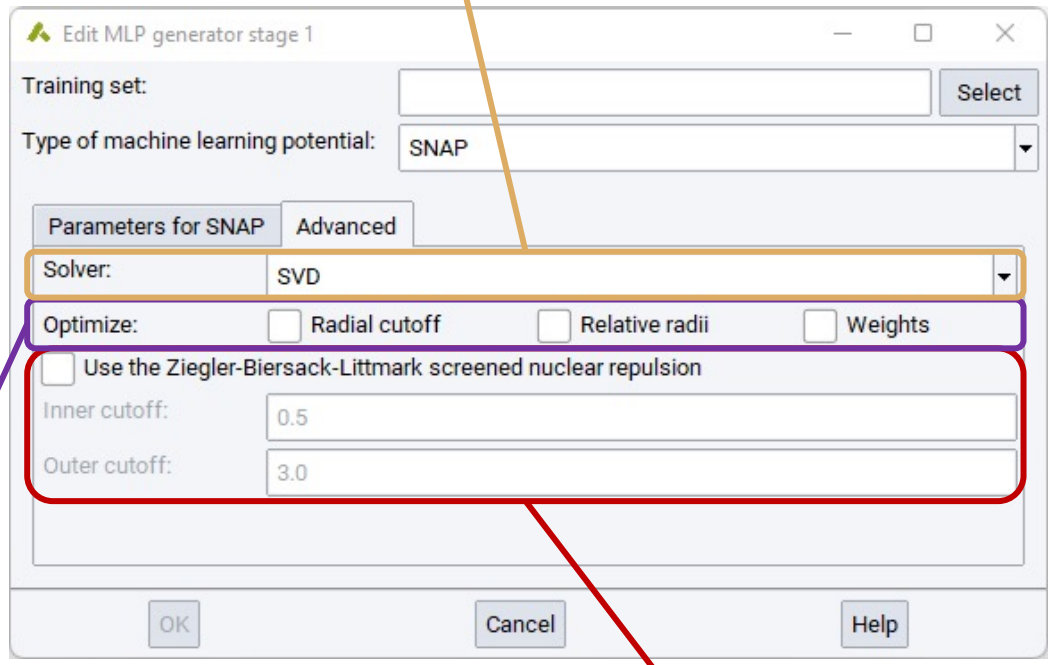
location of training set structure list



band limit = $2l$ (l = degree of spherical harmonics) - must be an even number

global radial cutoff r_C

linear regression solver for SNAP



fit energy, forces and/or stress?

respective fitting weights

for each element:

relative radius weight energy shift

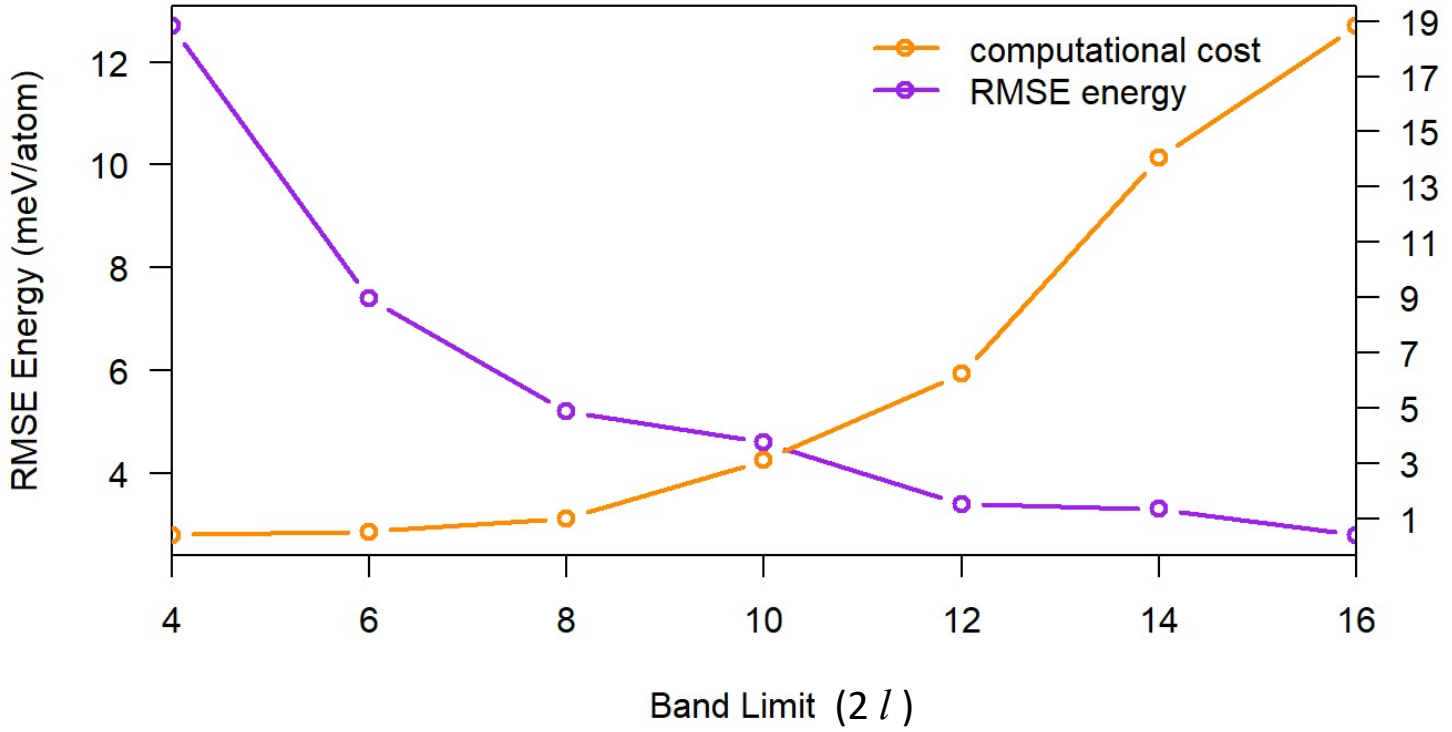
=> actual interaction radius: $(r_i + r_j)\, r_C$

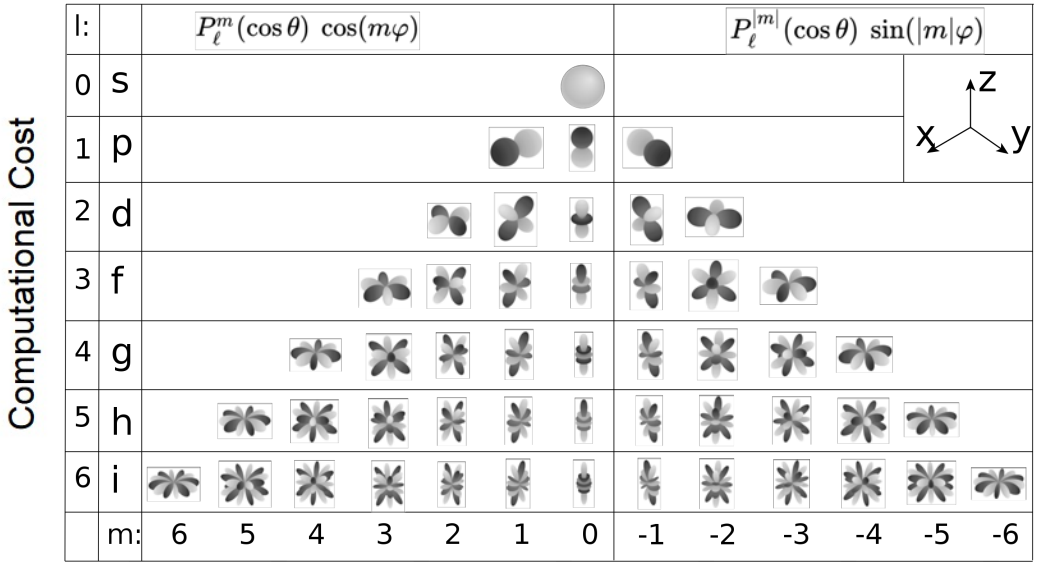
optimize respective hyper parameters (nonlinear)

ZBL settings

SNAP: Band Limit – Cost vs. Accuracy

Values based on 1 ps MD simulations at 300 K for a super cell with 54 Nb atoms.





Spherical harmonics Y_{lm} (© wikipedia.org)

- Accuracy decays exponentially
- Computational cost increases exponentially

Summary

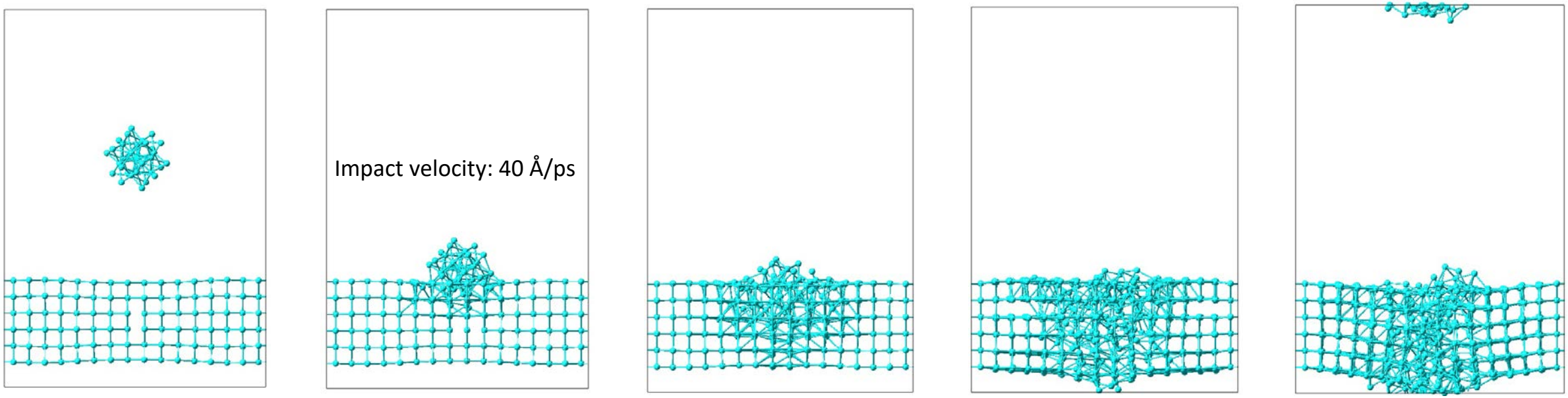
- Machine-learned potential as amplifier to calculate Nb cluster deposition on a Nb (110) surface based on *ab initio* accuracy

VASP

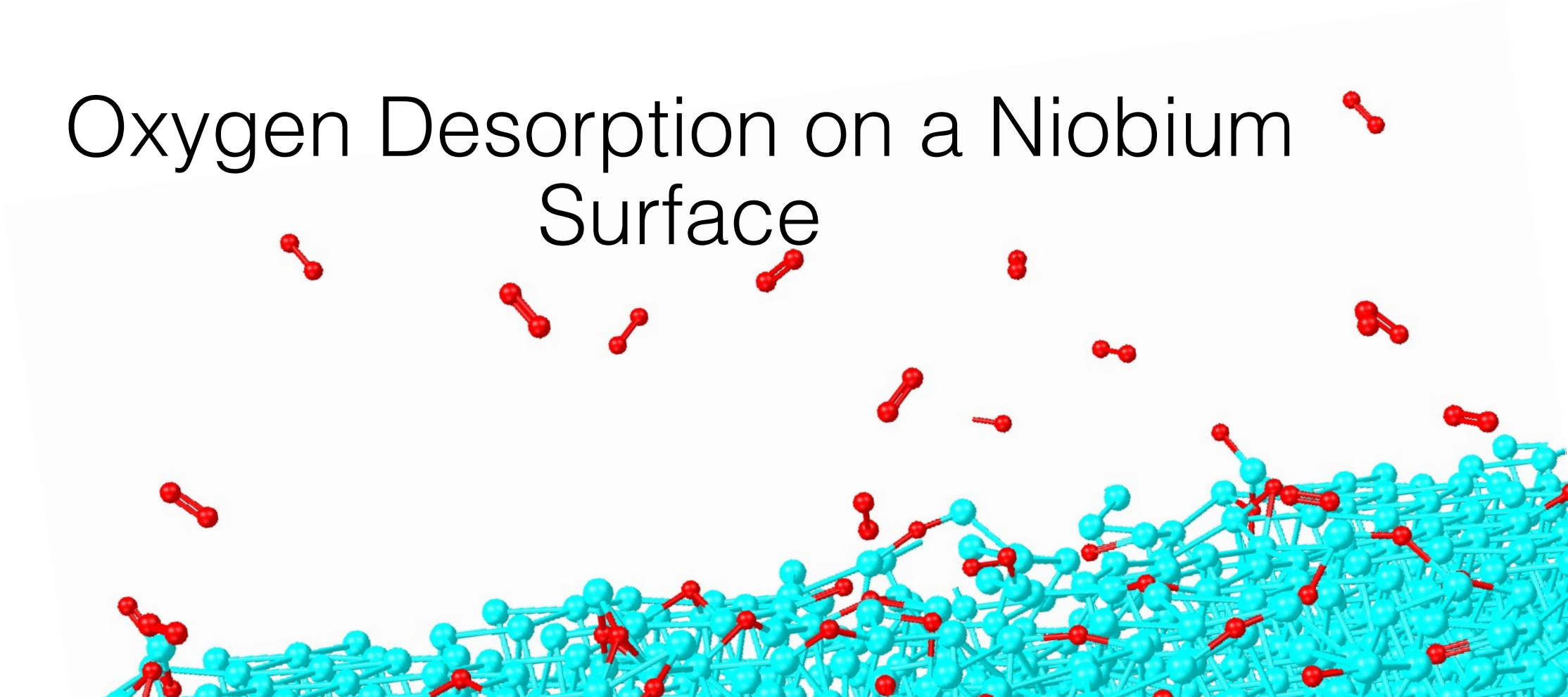
44 atoms, 100 frames

LAMMPS

809 atoms, 15000 frames

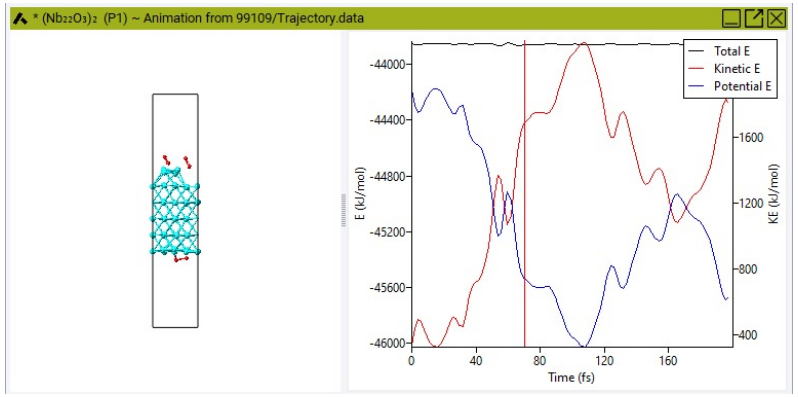


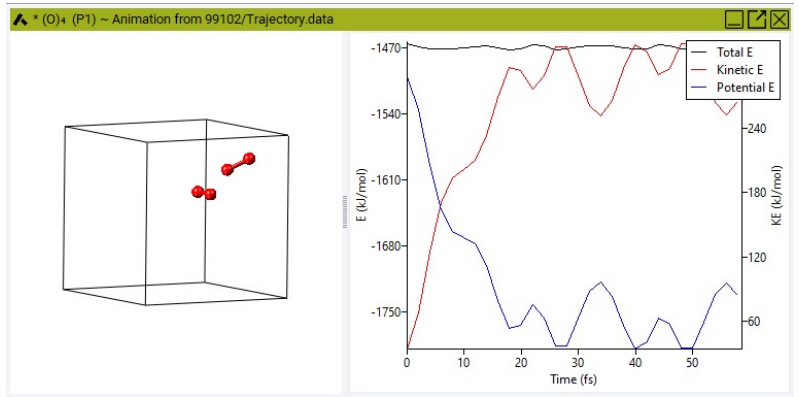
Oxygen Desorption on a Niobium Surface

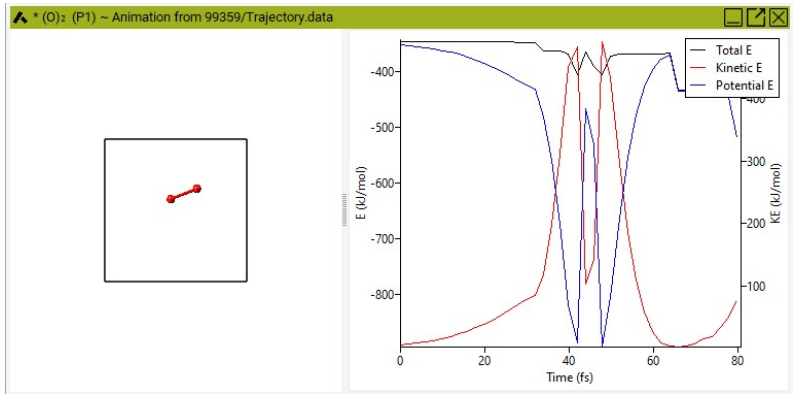


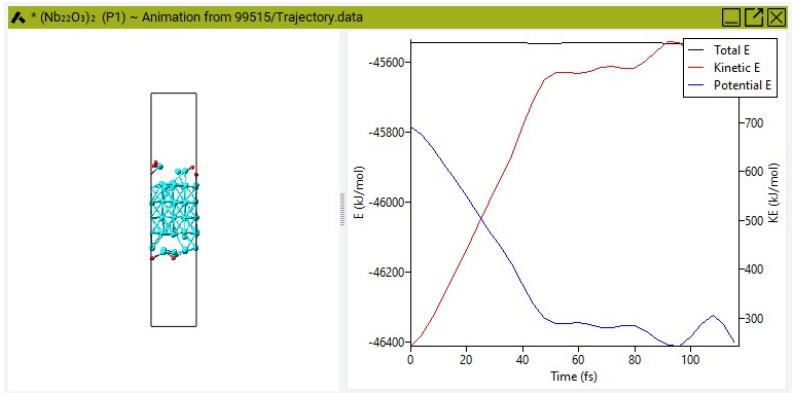
Procedure

- Extend the Nb surface slab training set to also consider the interaction with oxygen







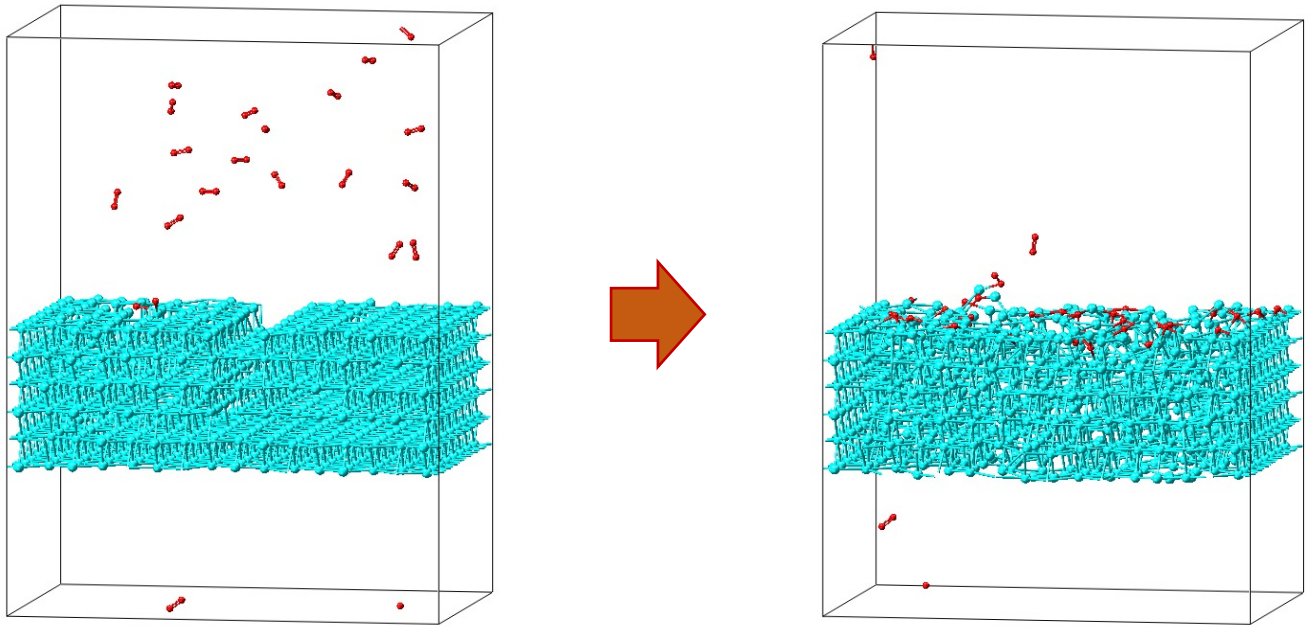


- Use VASP to run ab initio MD simulations (adjust time step and simulation length as appropriate)
  - **Calculation** tab
    Type of calculation: Molecular Dynamics, **Ensemble:** temperature scaling (nVE)
    Planewave cutoff: `350` **eV**, **Projection:** Real space
  - **Functional/Potential** tab: **Specific Potentials per Element** `O s`
  - **SCF** tab: **Spacing of k-points:** `0.4` 1/Ang, ☒ **Use odd size grids**, **Type of smearing:** Gaussian
- Use the MD trajectory to train a SNAP MLP
  - **Parameters for SNAP** tab
    Band limit: 12
  - **Advanced** tab
    Optimize ☒ **Radial cutoff** ☒ **Relative radii** ☒ **weights**

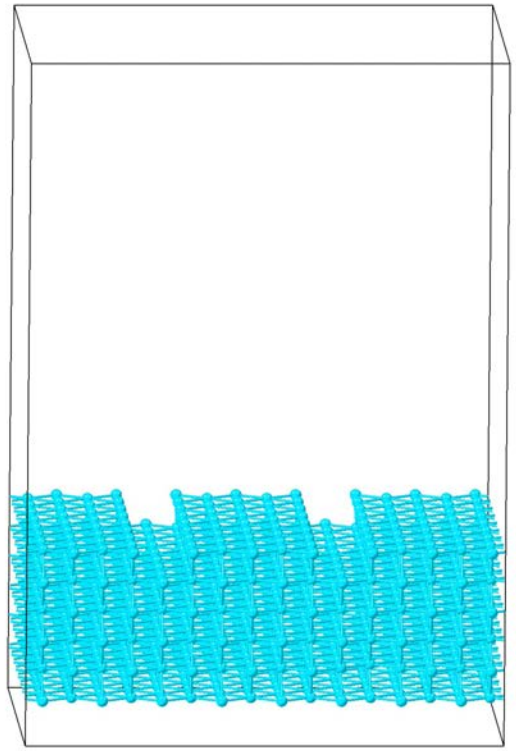
Training Set Creation → MLP Training → Apply the MLP

Summary

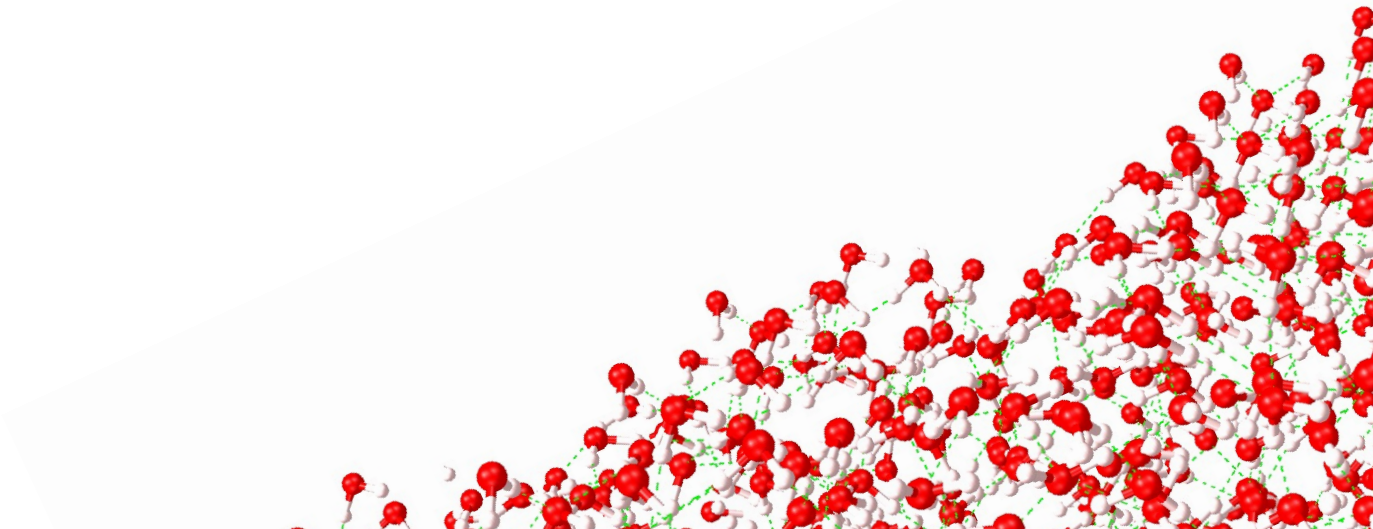
- Simulated the interaction of O_2 on a Nb (110) surface with a SNAP potential
  - Extended Nb training set with O_2, and Nb (110) + O_2 MD trajectories
  - MLP is a reactive forcefield – it can predict breaking and creation of O-O and Nb-O bonds
- Combine MLP with other *LAMMPS* modules such as *MedeA*



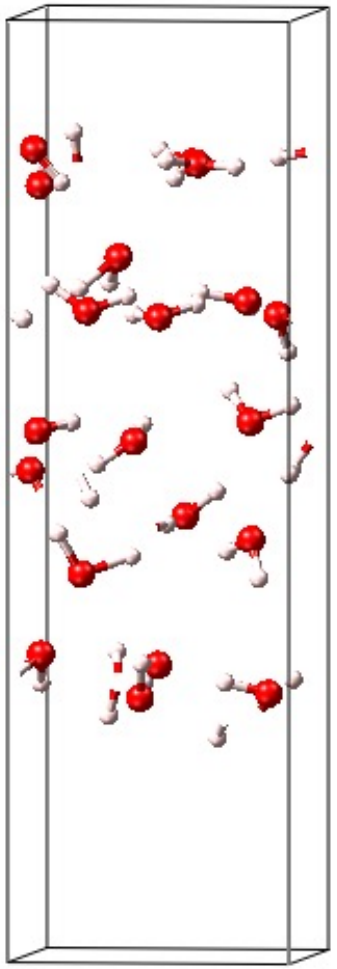
Deposition Simulation



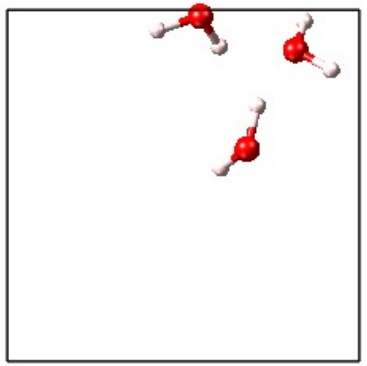
Water with Machine-Learned Potentials



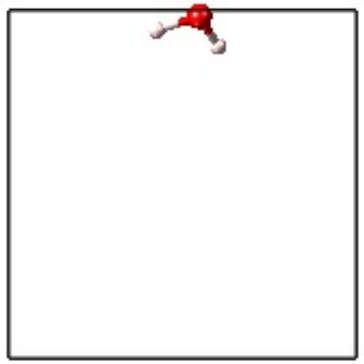
Procedure



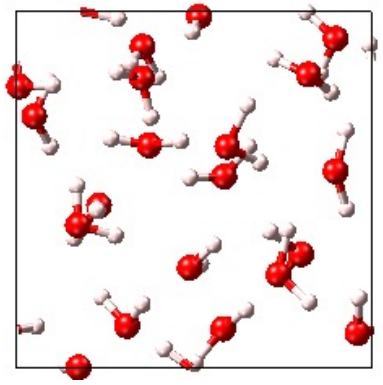
water slab



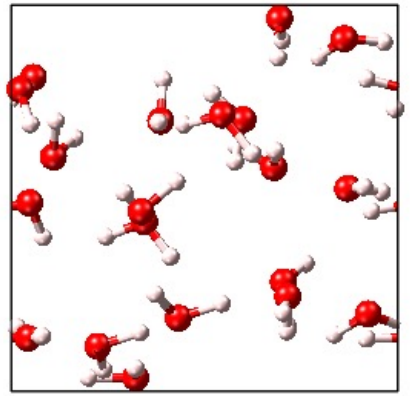
3 water molecules



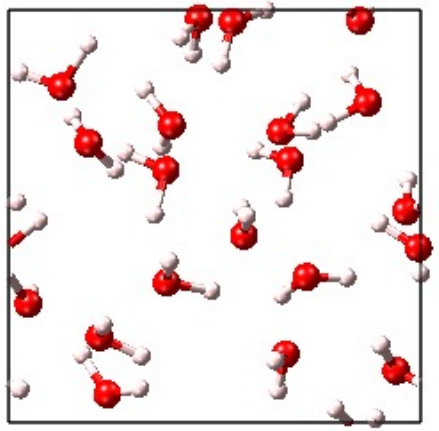
1 water molecules



ρ = 1100 kg/m^3



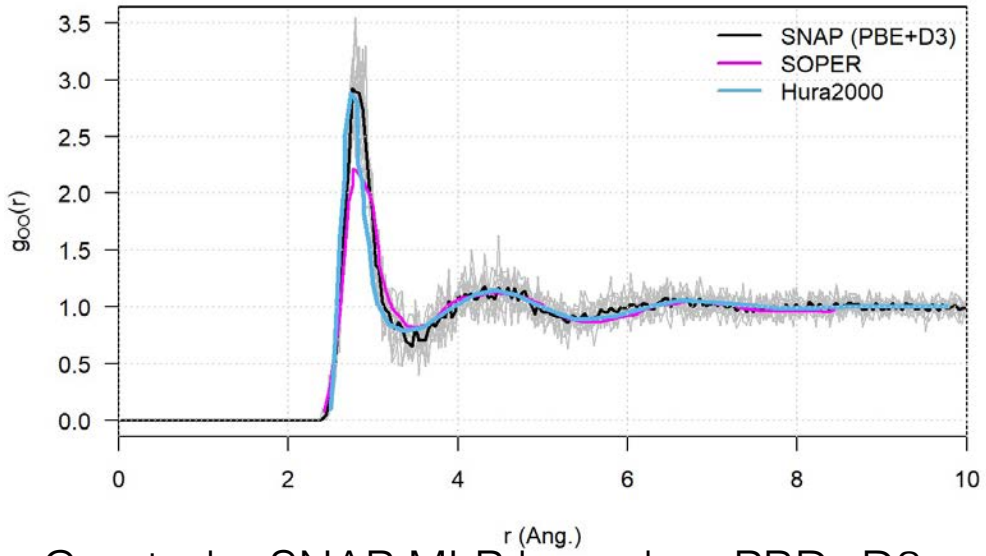
ρ = 1000 kg/m^3



ρ = 900 kg/m^3

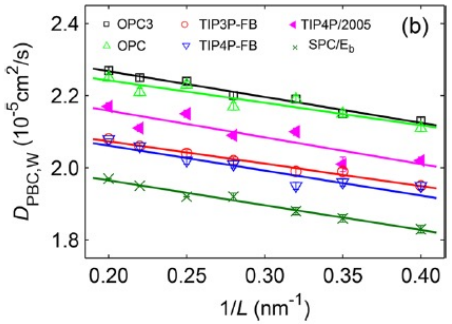
- Use VASP to run ab initio MD simulations (adjust time step and simulation length as appropriate)
  - **Calculation** tab
    Type of calculation: Molecular Dynamics, **Ensemble:** micro canonical (nVE), **Temperature initial:** 298 K
    Van der Waals: DFT-D3 zero-damping **Precision:** `Standard 500`
  - **SCF** tab
    Spacing of k-points: `0.2` 1/Ang, ☒ **Use odd size grids**, **Type of smearing:** Gaussian
- Use the MD trajectory to train a SNAP MLP
  - **Parameters for SNAP** tab
    Band limit: 12
  - **Advanced** tab
    Optimize ☒ **Radial cutoff** ☒ **Relative radii** ☒ **weights**

Summary



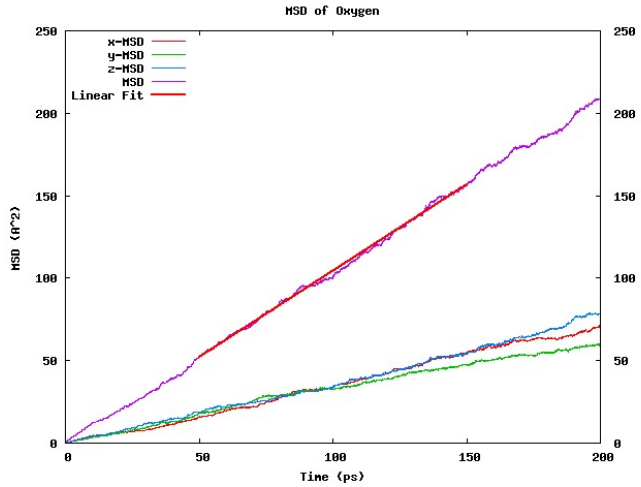
	$D_{O,W}$ (10^{-5}cm^2/s)	γ (mN/m)
SPC	4.52 (0.03) *	49.5 (0.3)
SPC/Eb	2.10 (0.02) *	60.4 (0.3)
TIP3P	6.14 (0.05) *	45.9 (0.7)
TIP3P-FB	2.20 (0.01) *	59.8 (0.3)
TIP4P	3.86 (0.03) *	51.4 (0.6)
TIP4P/2005	2.31 (0.02) *	62.6 (0.6)
TIP5P	2.93 (0.03) *	47.9 (0.6)
SNAP (PBE+D3)	**1.74** +	**47.0 (20)**
exp.	**2.299**	**71.99**

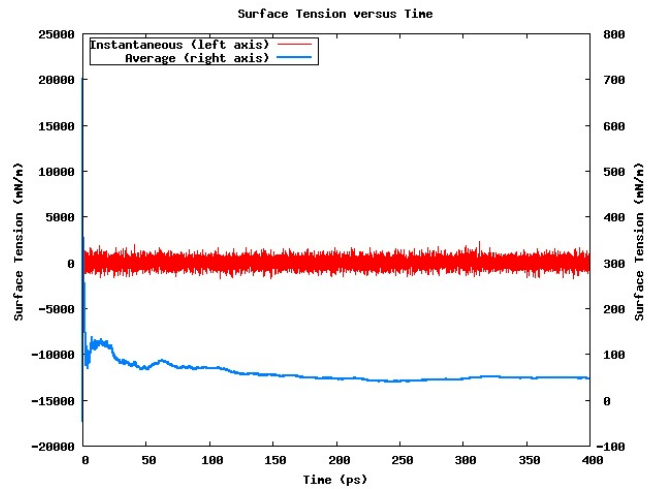
* value extrapolated for cell length to ∞, + cell length 2.29 nm



H. Zhang et al., J. Chem. Inf. Model. **58**, 1037−1052 (2018)

- Created a SNAP MLP based on PBD+D3
  - Excellent $g_{OO}(r)$ agreement with exp.
  - Good agreement for water diffusion
  - Better surface tension due to larger gap in DFT MD?
  - Density (298.2K, 1atm): 991.6 kg/m^3
    exp.: 997 kg/m^3
  - H-O-H angle: 103.4° (4.3°)
    exp.: 104.45°
- SNAP MLP is reactive: proton hopping





Conclusion

Guidelines on MLP Creation

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General guidelines

Always ensure that all entries in the training set have been calculated with consistent VASP settings – *MedeA* will help you (Flowcharts, VASP GUI: “Restore from Job”)

- PAW potentials
- Functional
- K-spacing
- Planewave cutoff energy

Training set: include ab initio MD simulations at temperatures higher than the temperature range to which the MLP should be applied

Create the MLP for the region in phase space that is of interest

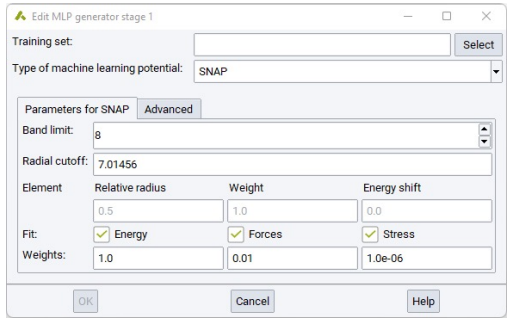
SNAP specific guidelines

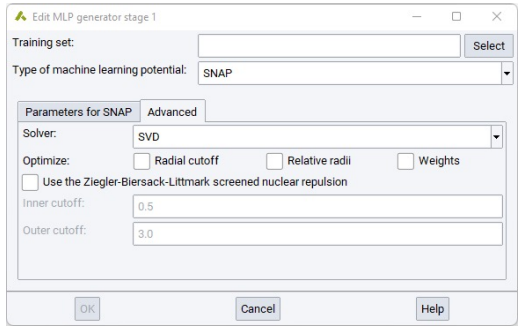
Use hyper-parameter optimization to optimize radial cutoff, relative radii and weights

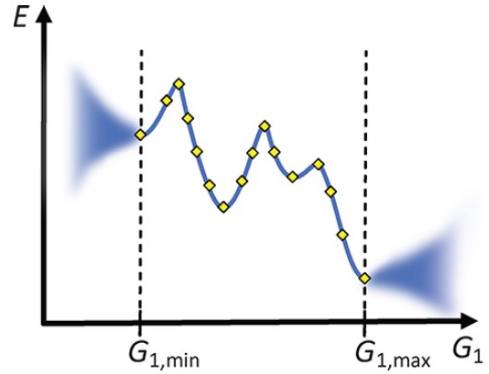
Balance band limit value between accuracy and speed (suggested range for this values lies between 8 to 12 – band limit = 2j)

Summary

- Demonstrated the use of the machine-learning potential generator to build MLPs from MD *ab initio* trajectories → bridging the length scale
  - Quality of the MLP depends on the training data – functional, accuracy etc.
  - Use Flowcharts to simplify the creation of your training set
  - MLPs interpolate *ab initio* data
- Machine-learned potentials are reactive as the examples Nb-O and water showed
- Machine-learned potentials can be used in *MedeA LAMMPS* like any other forcefield
  - Can be easily shared as an .frc file
  - Can make use of all the modules available to *MedeA LAMMPS*





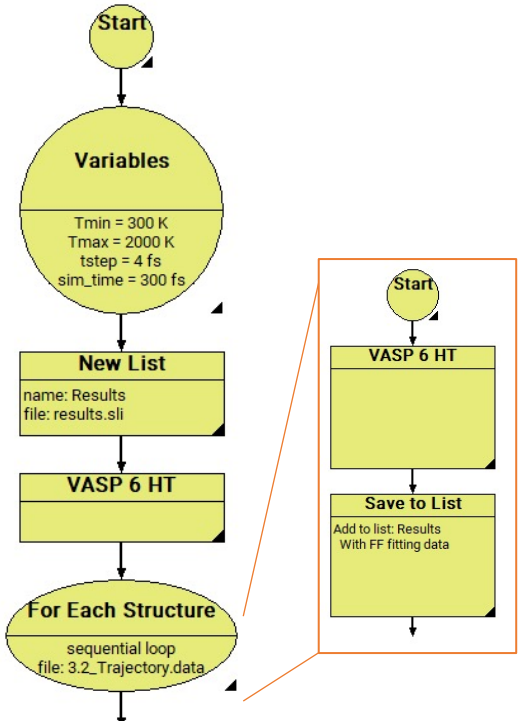


J. Behler, Chem. Rev. **121**, 10037–10072 (2021)

Define parameters for the MD simulation: lowest and highest temperature, time step, simulation time

Save results to the structure list **results.sli**

NPT MD simulation from $Tmin to $Tmax



MLPs with *MedeA LAMMPS*

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MedeA MT: Elastic, mechanical and thermodynamic properties (also at finite temperature)

MedeA Deformation: Perform deformation beyond the elastic regime

MedeA Thermal Conductivity: Calculate lattice thermal conductivity with Green Kubo or non-equilibrium MD Müller-Plathe

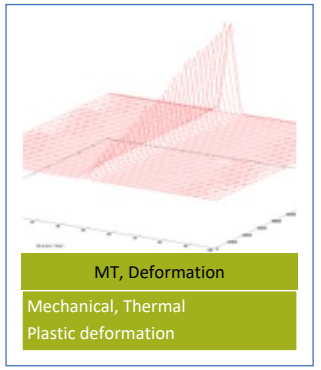
MedeA Viscosity: Calculate viscosity with Green Kubo or non-equilibrium MD Müller-Plathe

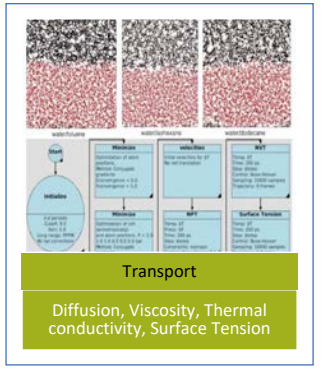
MedeA Surface Tension: Calculate surface tension of fluid slabs

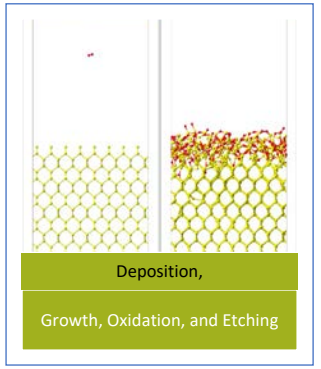
MedeA Diffusion: Automatically calculate diffusivity from mean square displacement

MedeA Deposition: Atomistic scale simulation to study deposition, growth, oxidation and etching

MedeA Phonon: Phonon spectra and thermodynamic functions (vibrational free energy, heat capacities)







List of Resources

Tutorials:

- **Introduction to MedeA MLP:** Machine learned potentials: Learn how to run LAMMPS simulations with machine-learned potentials
- **Introduction to MedeA MLPG:** Machine learned potential generator: Learn how to generate machine learned potentials with MedeA MLPG

Webinars:

- **MedeA Deposition:** Atomistic-Scale Simulations of Deposition, Growth, Oxidation, and Etching at your Fingertips
- Harness the Power of LAMMPS Molecular Dynamics Code with MedeA
- Classical Forcefields for Modeling Materials on Atomic Scale

Questions on Materials Design UGM Trainings

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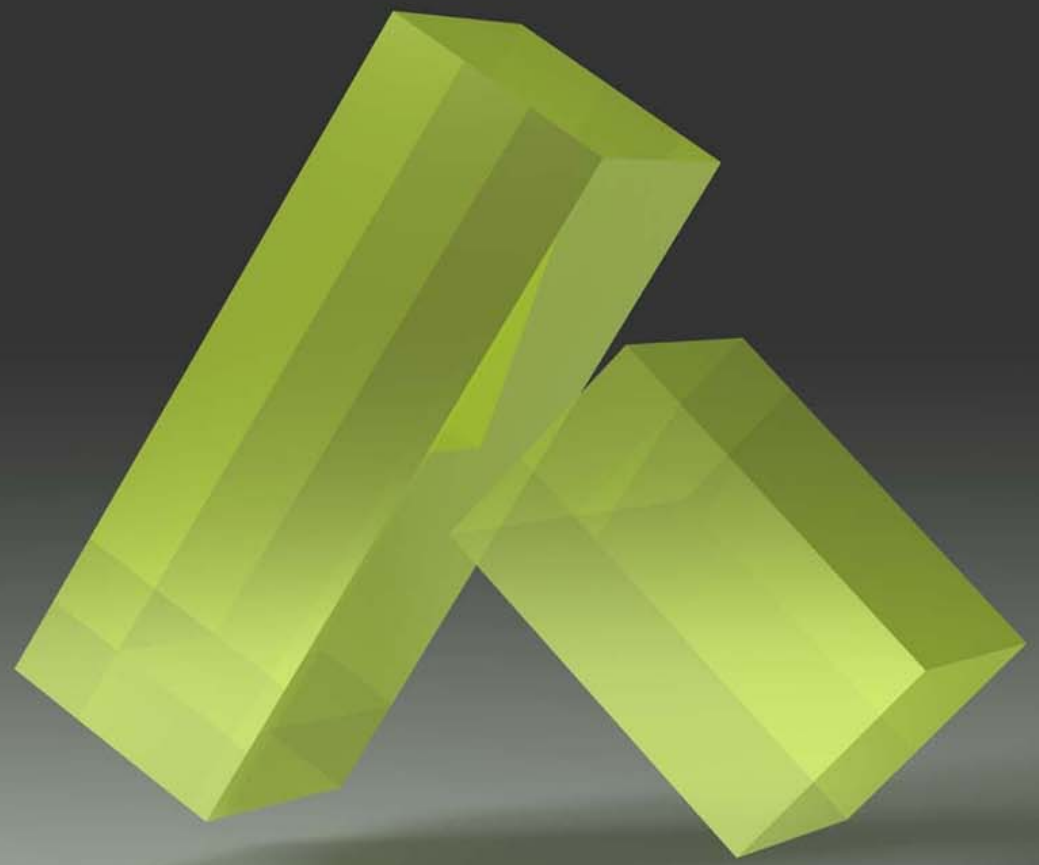
Question and Answer Session

David Reith

Materials Design

Ray Shan

Materials Design



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Innovation by Simulation