

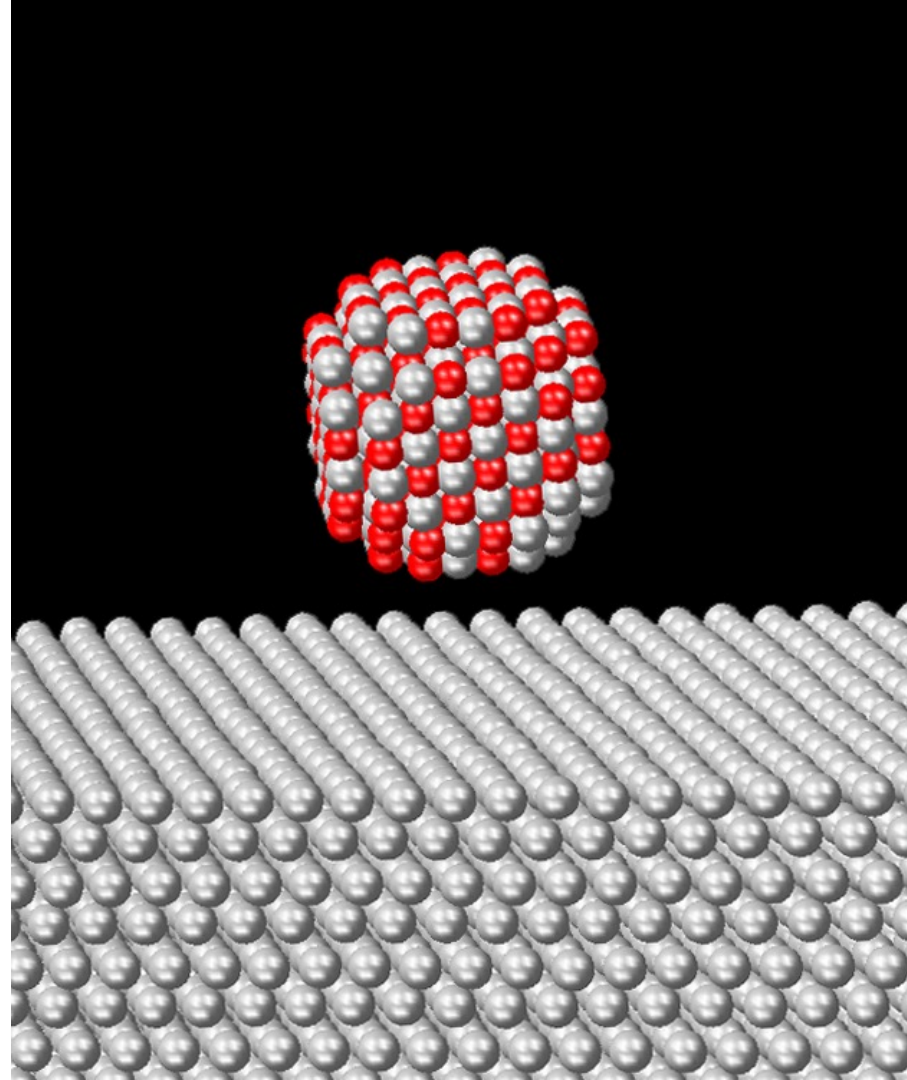


materials design

Ab initio for Millions

The Power of Machine-Learned
Potentials

December 7-9, 2021



Materials Design Webinar Series

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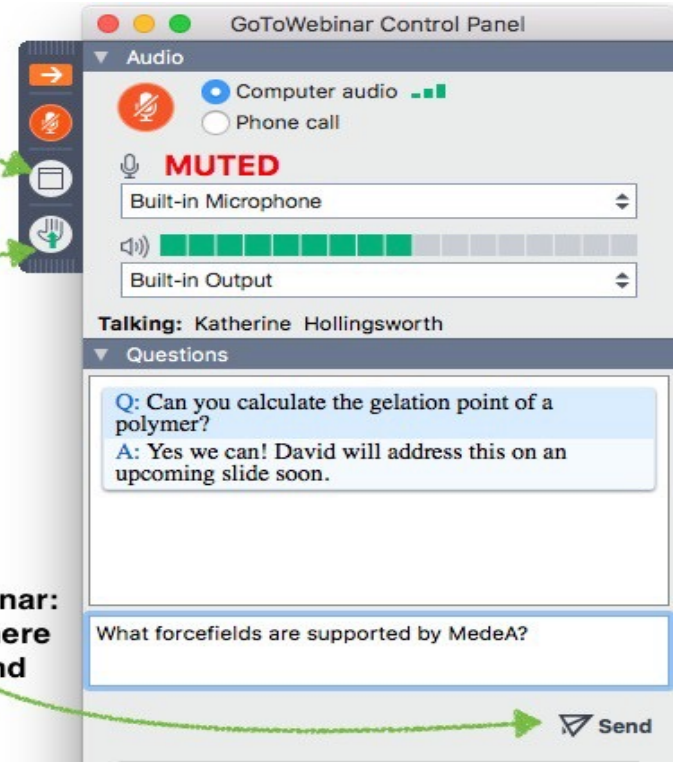
Please Ask Questions!

full screen

during discussion:
raise hand
to speak

Use the raise hand icon to bring
attention to your question

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type your question here
and then press Send





Webinar Speakers

Katherine Hollingsworth

Volker Eyert

Erich Wimmer

David Reith

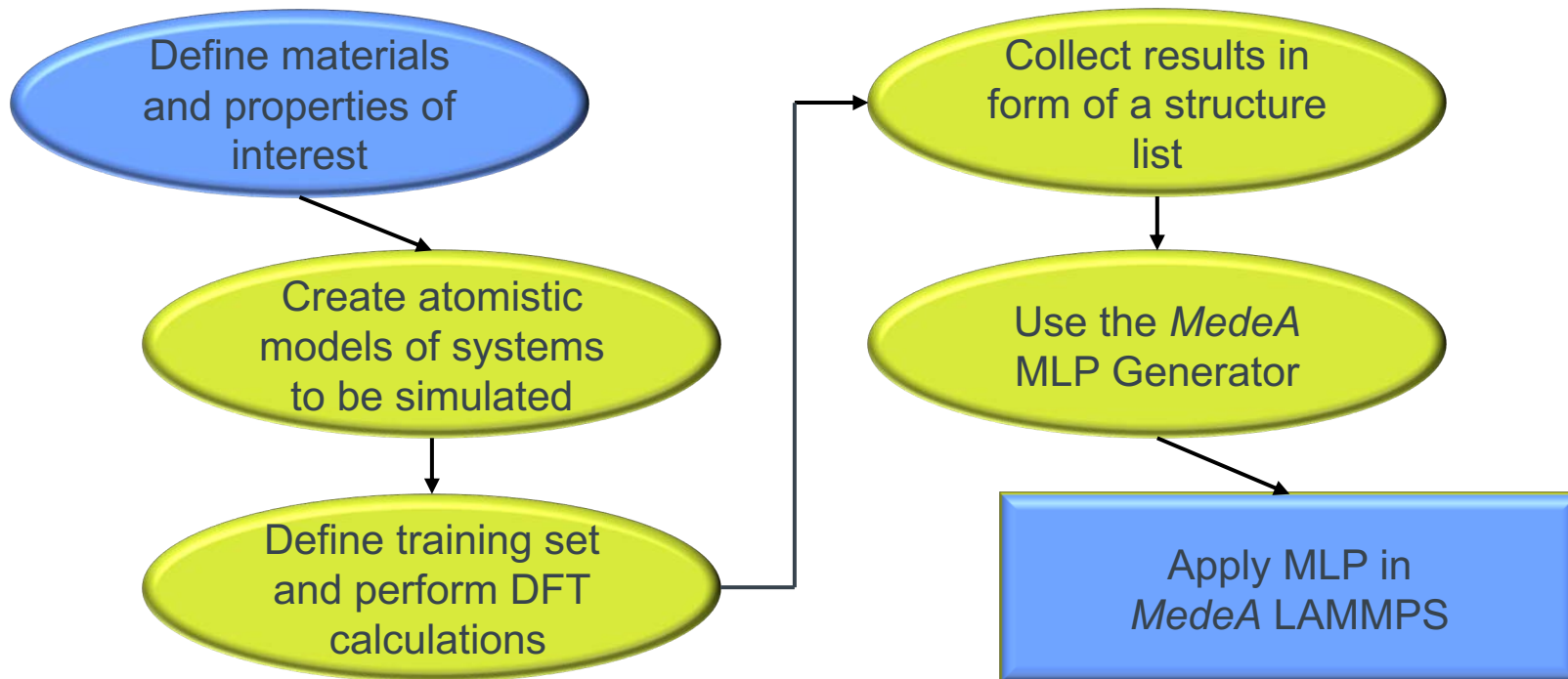
Agenda

- Introduction
- Applications
 - Phase Transitions of Titanium
 - AlN – Thermal Conductivity
 - Water – The Accuracy of MLPs
 - SiO₂ Polymorphs – One for All
 - Impact of Iodine on Zirconium
- Concluding Remarks
- Q&A

Impact of MgO Nanoparticle on Mg Slab

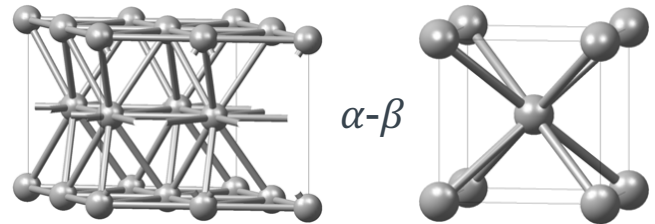
Molecular Dynamics Simulation using a
Machine-Learned Potential generated with
MedeA MLPG

Generating MLPs in *MedeA*: Workflow



Titanium

Explore α - β Phase Transition of Ti with SNAP



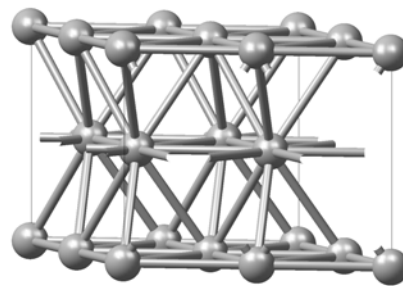
Training Set Calculations

Training set structures

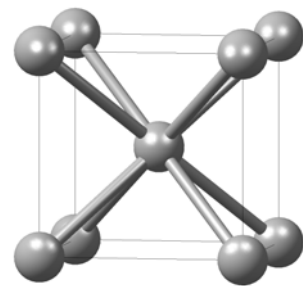
- Initial structures, supercells
- Vacancies, self-interstitial atoms, surfaces, stacking faults
- Isotropic and uniaxial strain by $\pm 0.5\%$, $\pm 1\%$, $\pm 1.5\%$, $\pm 2\%$, $\pm 4\%$, and $\pm 6\%$
- Angular deformations by 0.5° , 1° , and 2°
- NPT/NVT MD simulations at 300-1700 K
- Total of 1005 structures

VASP computational parameters

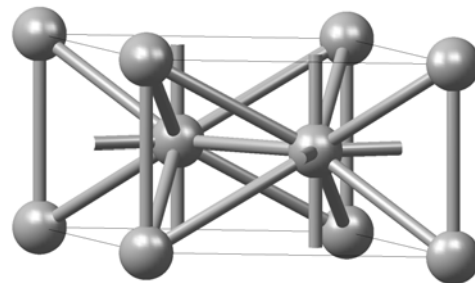
- PBE functional
- 520 eV plane-wave cutoff
- **k**-point spacing 0.2 \AA^{-1}



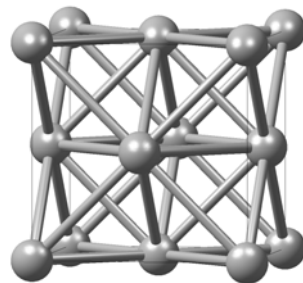
α -phase, hcp
 $3 \times 3 \times 2$ supercell



β -phase, bcc
 $3 \times 3 \times 3$ supercell

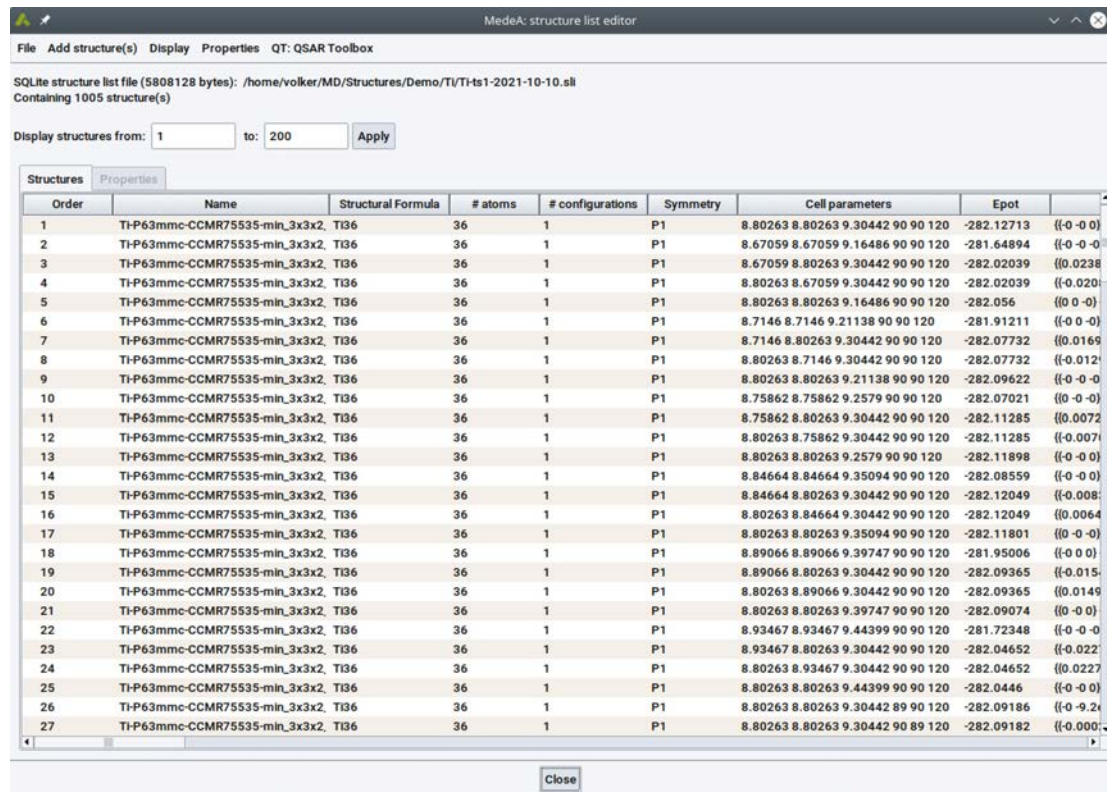


ω -phase, hex
 $2 \times 2 \times 3$ supercell



fcc
 $2 \times 2 \times 2$ supercell

MedeA MLP Generator: Prepare



The screenshot shows the 'MedeA: structure list editor' window. The title bar includes a file icon, a search icon, and window controls. The menu bar contains 'File', 'Add structure(s)', 'Display', 'Properties', and 'QT: QSAR Toolbox'. The main text area displays the file path: 'SQLite structure list file (5808128 bytes): /home/volker/MD/Structures/Demo/TV/Th-ts1-2021-10-10.sli' and 'Containing 1005 structure(s)'. Below this, there are input fields for 'Display structures from: 1 to: 200' and an 'Apply' button. The main content is a table with columns: 'Order', 'Name', 'Structural Formula', '# atoms', '# configurations', 'Symmetry', 'Cell parameters', 'Epot', and a column with a double arrow icon. The table lists 27 structures, all with the name 'Ti-P63mmc-CCMR75535-min_3x3x2, Ti36'. The 'Cell parameters' column contains three sets of values (a, b, c) and the 'Epot' column contains energy values. The last column contains a double arrow icon.

Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters	Epot	
1	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.30442 90 90 120	-282.12713	{(-0 -0)}
2	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.67059 8.67059 9.16486 90 90 120	-281.64894	{(-0 -0)}
3	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.67059 8.80263 9.30442 90 90 120	-282.02039	{(0.0238}
4	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.67059 9.30442 90 90 120	-282.02039	{(-0.0202}
5	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.16486 90 90 120	-282.056	{(0 0 -0)}
6	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.7146 8.7146 9.21138 90 90 120	-281.91211	{(-0 0 -0)}
7	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.7146 8.80263 9.30442 90 90 120	-282.07732	{(0.0169}
8	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.7146 9.30442 90 90 120	-282.07732	{(-0.0121}
9	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.21138 90 90 120	-282.09622	{(-0 -0 -0)}
10	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.75862 8.75862 9.2579 90 90 120	-282.07021	{(0 -0 -0)}
11	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.75862 8.80263 9.30442 90 90 120	-282.11285	{(0.0072}
12	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.75862 9.30442 90 90 120	-282.11285	{(-0.0071}
13	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.2579 90 90 120	-282.11898	{(-0 -0 -0)}
14	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.84664 8.84664 9.35094 90 90 120	-282.08559	{(-0 -0 -0)}
15	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.84664 8.80263 9.30442 90 90 120	-282.12049	{(-0.0081}
16	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.84664 9.30442 90 90 120	-282.12049	{(0.0064}
17	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.35094 90 90 120	-282.11801	{(0 -0 -0)}
18	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.89066 8.89066 9.39747 90 90 120	-281.95006	{(-0 0 0)}
19	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.89066 8.80263 9.30442 90 90 120	-282.09365	{(-0.0151}
20	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.89066 9.30442 90 90 120	-282.09365	{(0.0149}
21	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.39747 90 90 120	-282.09074	{(0 -0 -0)}
22	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.93467 8.93467 9.44399 90 90 120	-281.72348	{(-0 -0 -0)}
23	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.93467 8.80263 9.30442 90 90 120	-282.04652	{(-0.0221}
24	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.93467 9.30442 90 90 120	-282.04652	{(0.0227}
25	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.44399 90 90 120	-282.0446	{(-0 -0 -0)}
26	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.30442 89 90 120	-282.09186	{(-0 -9.24}
27	Ti-P63mmc-CCMR75535-min_3x3x2, Ti36		36	1	P1	8.80263 8.80263 9.30442 90 89 120	-282.09182	{(-0.0001}

Collect information about training set in structure list

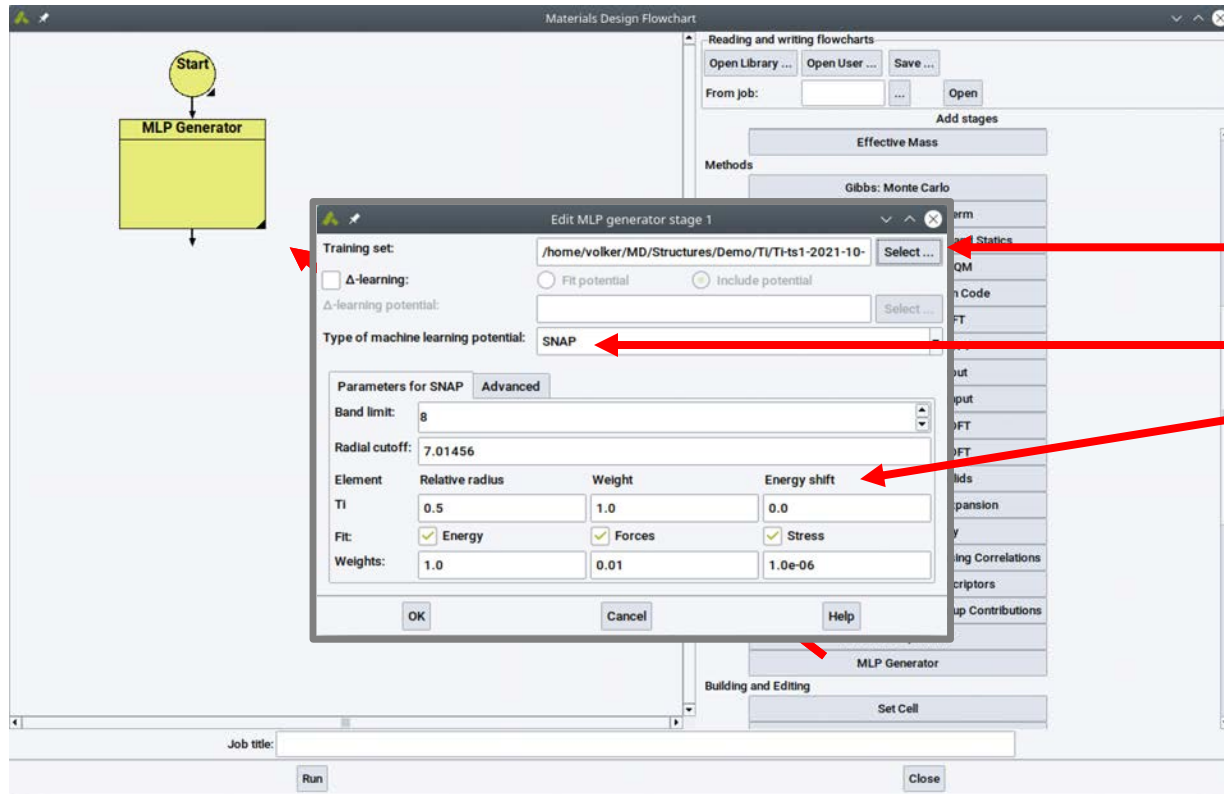
- Structures
- Energies
- Forces
- Stresses

MedeA MLP Generator: Start

The screenshot displays the 'Materials Design Flowchart' application. On the left, a flowchart shows a 'Start' node (yellow circle) with an arrow pointing to an 'MLP Generator' node (yellow rectangle). A red arrow originates from the 'MLP Generator' node in the flowchart and points to the 'MLP Generator' option in the 'Methods' list on the right. The 'Methods' list is a scrollable area containing various computational methods, including 'Effective Mass', 'Gibbs: Monte Carlo', 'Gibbs: Adsorption Isotherm', 'LAMMPS: Molecular Dynamics and Statics', 'MOPAC: Semiempirical QM', 'Gaussian: Ab Initio Gaussian Code', 'VASP 6: Plane Wave DFT', 'VASP 5.4: Plane Wave DFT', 'VASP 6: High Throughput', 'VASP 5.4: High Throughput', 'VASP 5.2: Plane Wave DFT', 'VASP 4.6: Plane Wave DFT', 'Phonon: Vibrations in Solids', 'UNCLE: UNiversal CLuster Expansion', 'UNCLE: Save Property', 'P3C: Polymer Property Prediction using Correlations', 'Descriptors: Get MedeA descriptors', 'GPR: Property Prediction using Group Contributions', 'Forcefield Optimizer', and 'MLP Generator'. Below the 'Methods' list is a 'Building and Editing' section with a 'Set Cell' button. At the bottom of the window, there is a 'Job title:' field, a 'Run' button, and a 'Close' button.

Call MLP Generator in Flowchart

MedeA MLP Generator: Specify

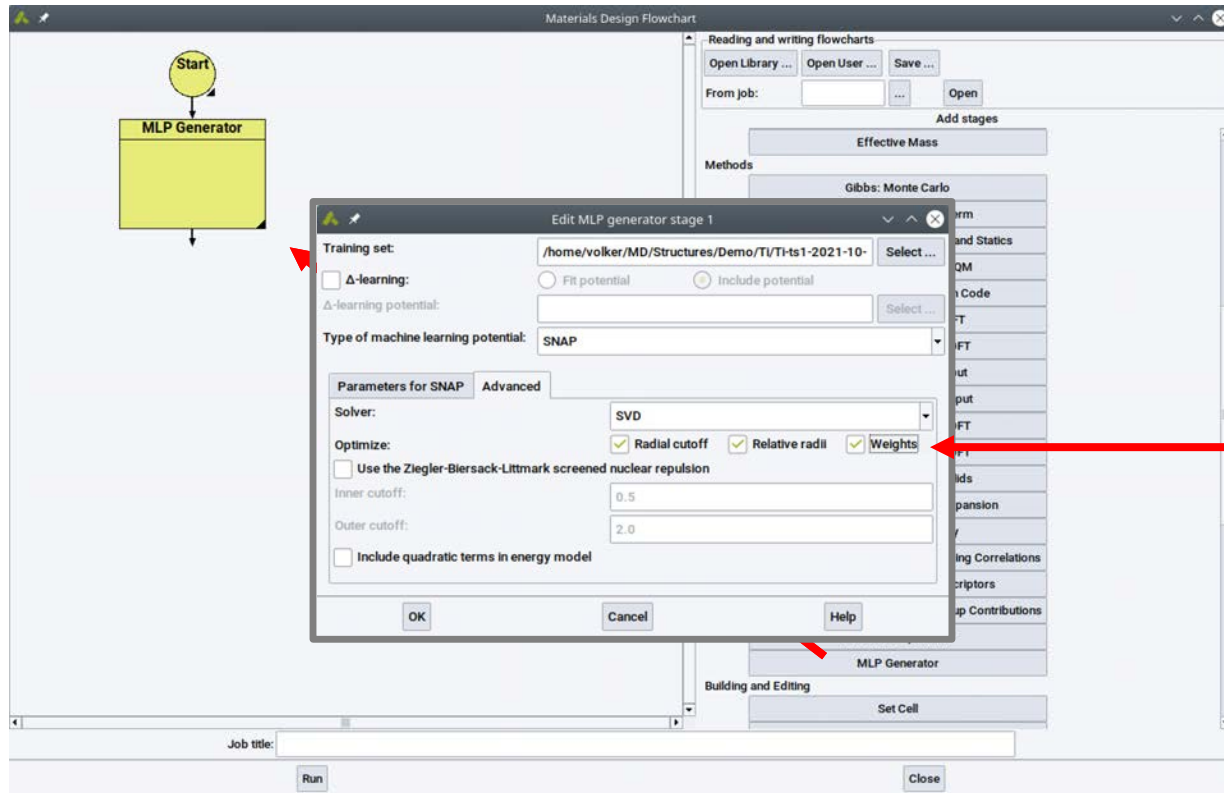


Call MLP Generator in Flowchart

Specify

- Training set, i.e, structure list
- Type of potential
- Basic parameters

MedeA MLP Generator: Finetune



Call MLP Generator in Flowchart

Specify

- Training set, i.e, structure list
- Type of potential
- Basic parameters
- Advanced settings

MedeA MLP Generator: Analyze

Stage 1: MLP Generator

Input for FitSNAP is in "Ti-tsl-2021-10-10.in":

```
Band limit: 10
Radial cutoff: 7.01456 Ang
Elements:
```

	Rel. radius	Weight	Energy shift
Ti	1.0000	0.5000	0.000000

Properties used in the fit: energy forces stress
with weights: 1.0 0.05 1.0e-05

The Ziegler-Biersack-Littmark screened nuclear repulsion with inner/outer radius of 0.5/2.0 Ang is being used.

The following parameters are optimized during the MLP generator run:

Parameter	Initial	Optimized
Radial cutoff	7.01456	6.02630
Relative radius for Ti	0.50000	0.59345
Weight for Ti	1.00000	1.00917

Fitting statistics

Group	Weighting	Subsystem	Count	Mean absolute error	Root mean absolute error	Root mean squared error	Relative root mean squared error	R squared
all	Unweighted	Combined	127401	59.9335	0.0739	487.8104	0.0586	0.9966
all	Unweighted	Energy	1005	0.0133	0.1452	0.0178	0.1341	0.9820
all	Unweighted	Forces	120366	0.0583	0.3595	0.1091	0.2428	0.9411
all	Unweighted	Stress	6030	1265.1000	0.0738	2242.2232	0.0586	0.9966
all	Weighted	Combined	127401	0.0035	0.0453	0.0074	0.0108	0.9999
all	Weighted	Energy	1005	0.0133	0.1452	0.0178	0.1341	0.9820
all	Weighted	Forces	120366	0.0029	0.3595	0.0055	0.2428	0.9411
all	Weighted	Stress	6030	0.0127	0.0738	0.0224	0.0586	0.9966

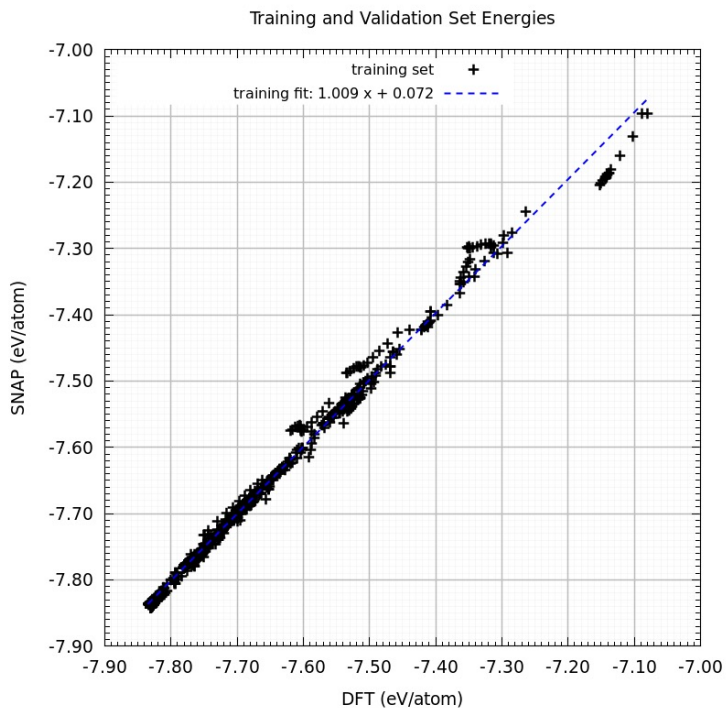
Units: energy: eV/atom, force: eV/Angstrom, pressure: bar

Generated SNAP has been converted to "/data/medea/ContractJobs/dir97000/97338/Stage_1/Ti-tsl-2021-10-10.frc".

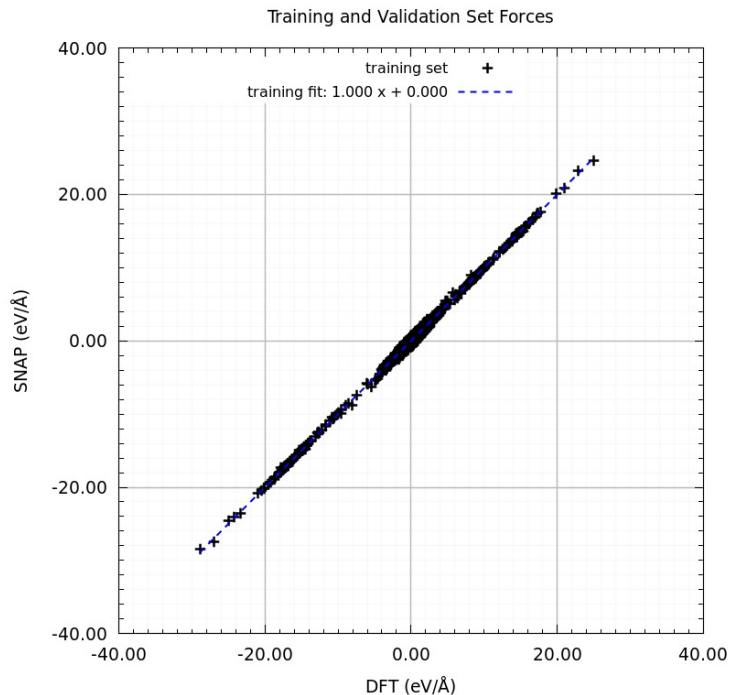
Information in Job.out

- Type of potential (SNAP, NNP)
- (Optimized) parameters
- Fitting statistics
- Pointer to generated MLP

MedeA MLP Generator: Assess

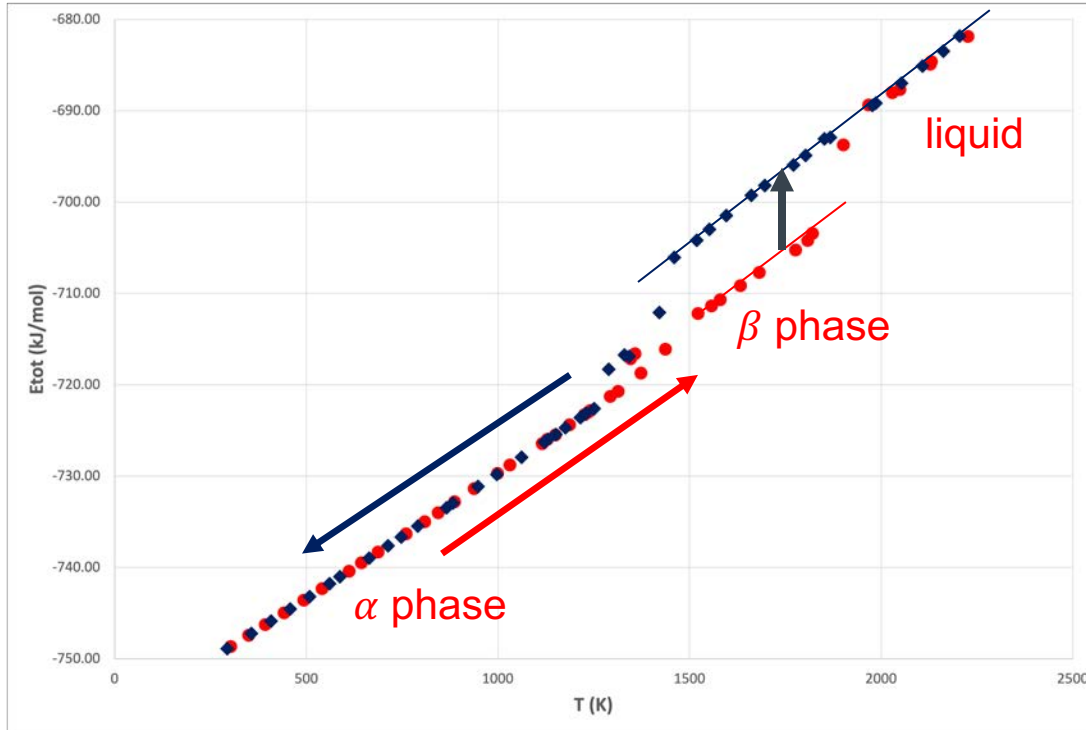


Energies



Forces

Ti: α - β Phase Transition



CCMR 109654, 109657

Transition temperatures (exp):

- α - β transition: 1156 K
- melting: 1946 K

Latent heat of α - β transition:

- MLP: $\Delta H = 2.7$ kJ/mol
- Exp.: $\Delta H = 4.3$ kJ/mol

Heat of fusion:

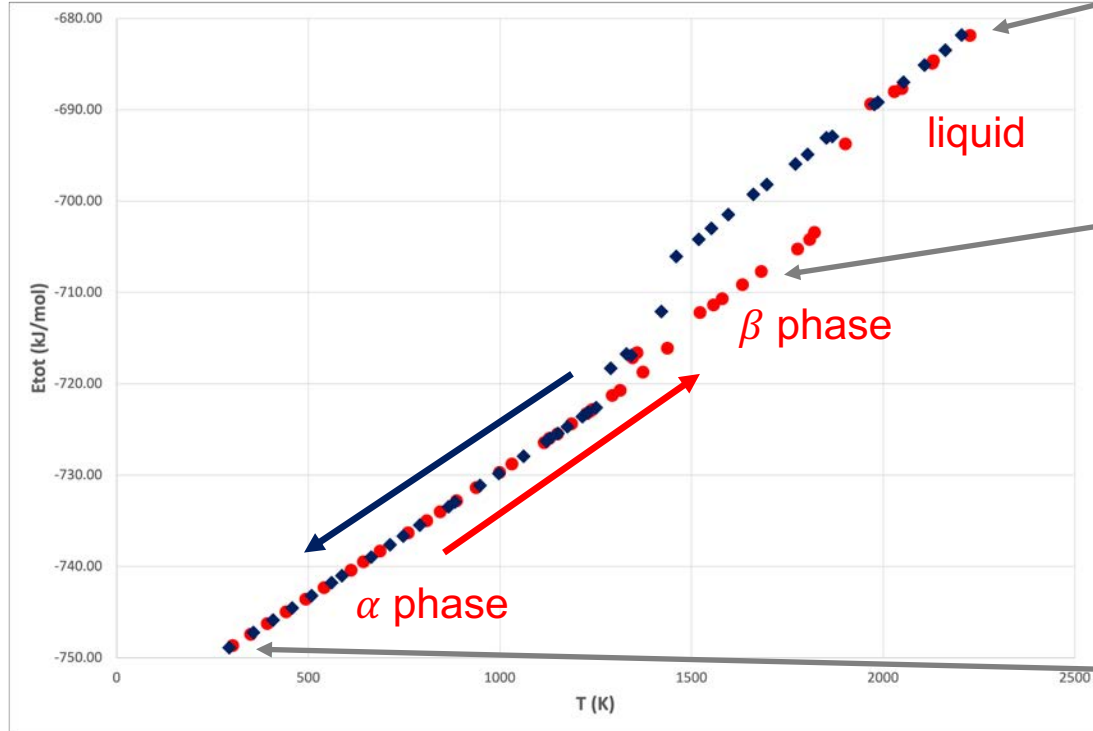
- MLP: $\Delta H = 10.4$ kJ/mol
- Exp.: $\Delta H = 13$ kJ/mol

Specific heat:

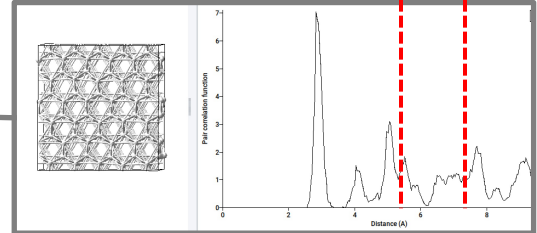
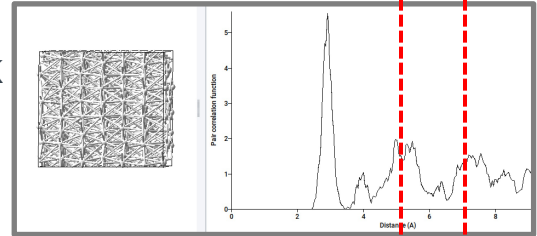
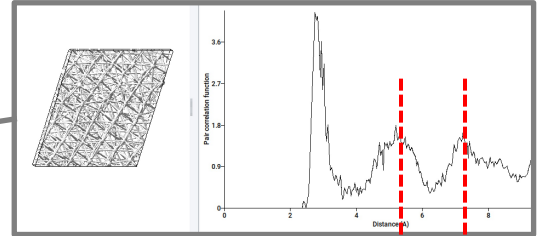
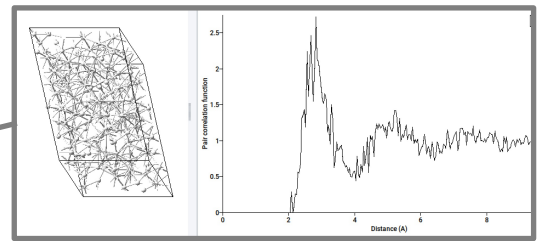
- MLP: $c_p = 28$ - 30 J/(mol·K)
- Exp.: $c_p = 25$ - 37 J/(mol·K)

McClure et al., Int. J. Thermophys. **13**, 75 (1992), Kaschnitz et al., J. Therm. Anal. Calorim. **64**, 351 (2001), Int. J. Thermophys. **23**, 1339 (2002)

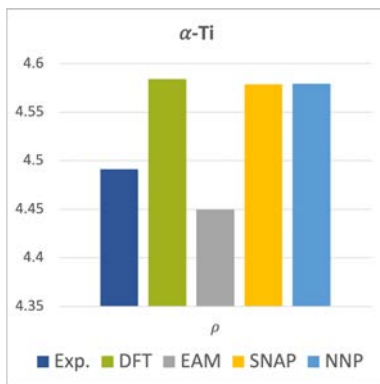
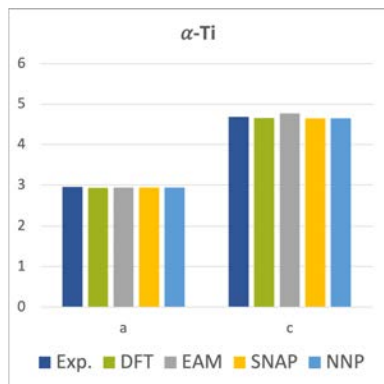
Ti: α - β Phase Transition



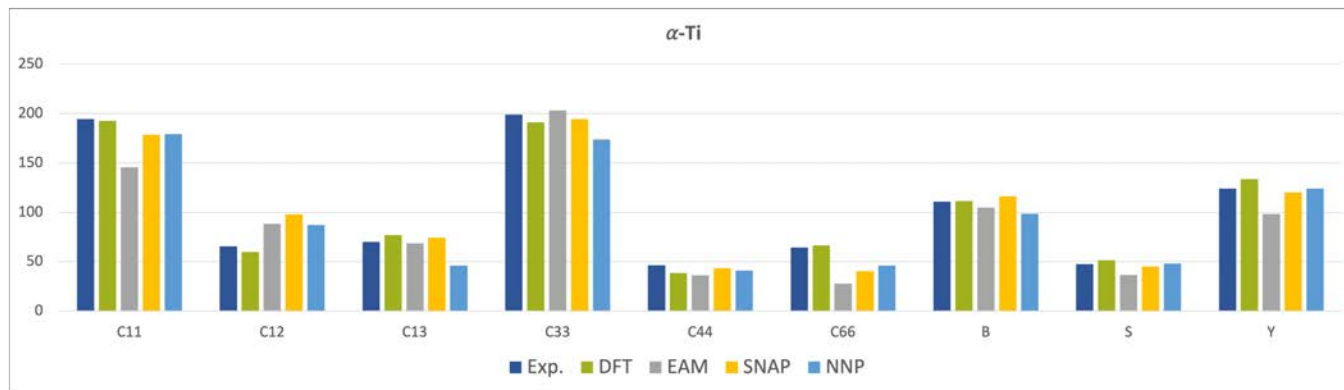
β phase at 300 K



α -Ti: Equilibrium and Elastic Properties



DFT: *MedeA VASP*, EAM: Zhou et al., Francis et al., Exp.: P. D. Hao et al., *J. Mater. Res. Technol.* **9**, 3488 (2020)

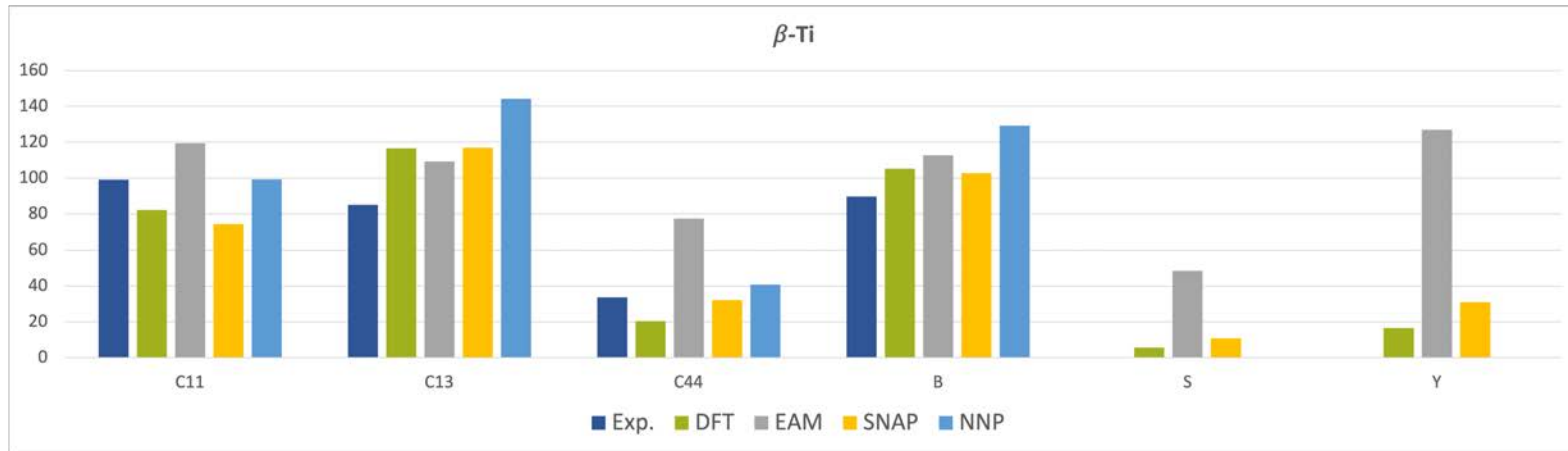


a, c in Å
 ρ in g/cm³
 C_{ij} in GPa

β -Ti: Equilibrium and Elastic Properties

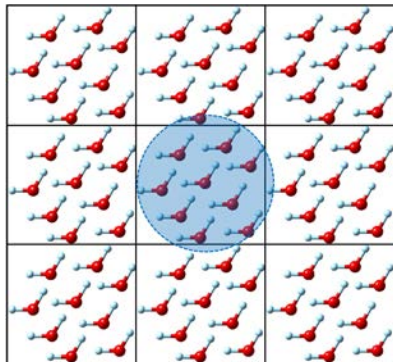


DFT: *MedeA* VASP, EAM: Zhou et al., Francis et al., Exp.^a: H. Ledbetter et al., *J. Appl. Phys.* **95**, 4642 (2004), Exp.^b: E. Fisher and D. Dever, *Science, Technology, and Application of Titanium* (Pergamon, NY 1970), p. 373



a, c in Å
 ρ in g/cm³
 C_{ij} in GPa

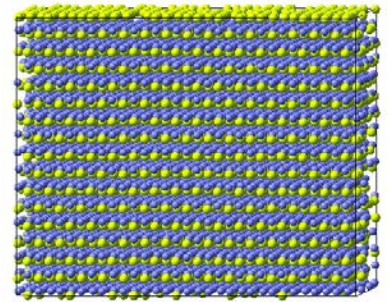
Approaches to MLPs



- Divide structure into local atomic environments/clusters **described** in terms of atom positions and types
 - Express energies/forces/stresses in terms of **local descriptors** of all clusters
 - Determine (train) parameters relating energies/forces stresses and local descriptors using *ab initio* calculations
-
- Spectral Neighbor Analysis Potential (SNAP)
 - A. Thompson and coworkers
 - FitSNAP code by A. Thompson *et al.*, Sandia
 - Neural Network Potential (NNP)
 - J. Behler and M. Parrinello
 - n2p2 code by A. Singraber, Univ. Vienna

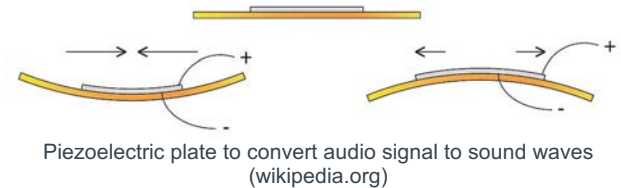
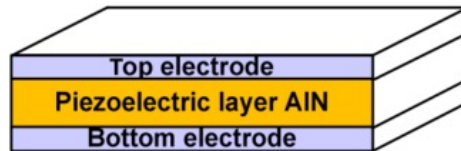
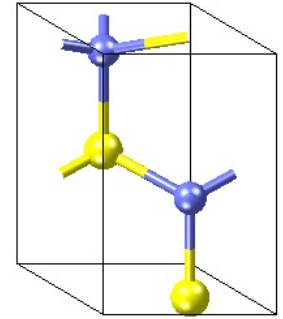
Thermal Conductivity

AlN in Wurtzite Structure



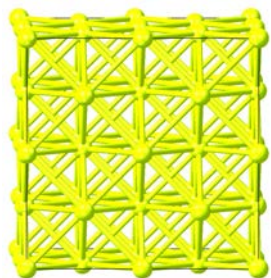
Industrial Application of Wurtzite Aluminum Nitride

- High thermal conductivity
 - Remove heat with an insulating material
- Good piezoelectric and acoustic properties
 - Thin film AlN on Si wafers used as surface acoustic wave sensors
 - Used as ultrasound transducers: emit and receive ultrasound
 - Acoustic resonator (resonance frequency = $\frac{v_{acoustic}}{2d}$) can be used as a radio frequency filter or a pressure sensor

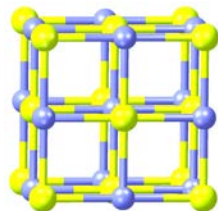


Training Set

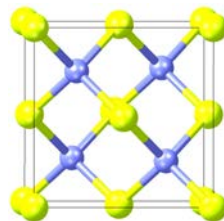
- NPT MD trajectory for 16 atoms and 96 atoms wurtzite AlN supercell
 - Temperatures: 150 K, 300 K, 600 K, 1500 K
- Strained Al-N structures: wurtzite, rocksalt, zinc blende
- NVT MD trajectories of (001) and (110) wurtzite AlN surface slabs
- NPT MD trajectory for a 32 atoms fcc Al supercell
 - Temperature: 300 K to 1000 K
- Total number of structures in training set: 431



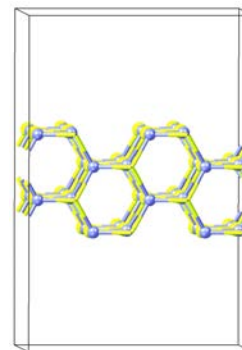
32 atoms fcc Al



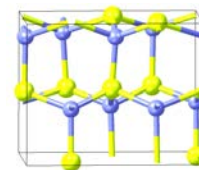
AlN rocksalt



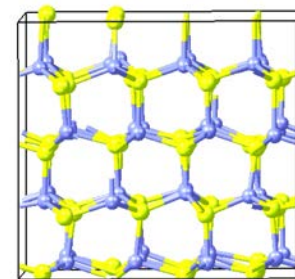
AlN zinc blende



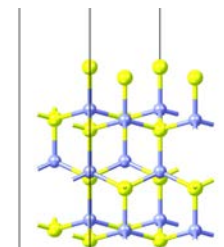
AlN (110) surface slab



16 atoms wurtzite AlN



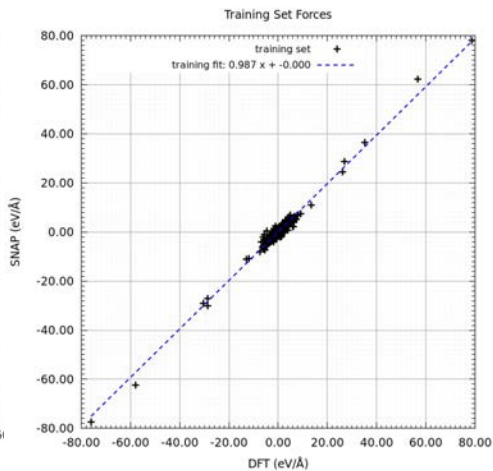
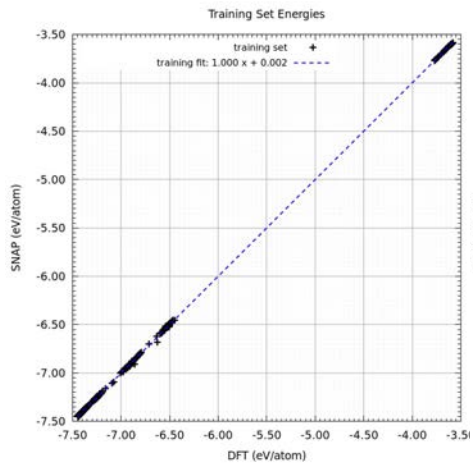
96 atoms wurtzite AlN



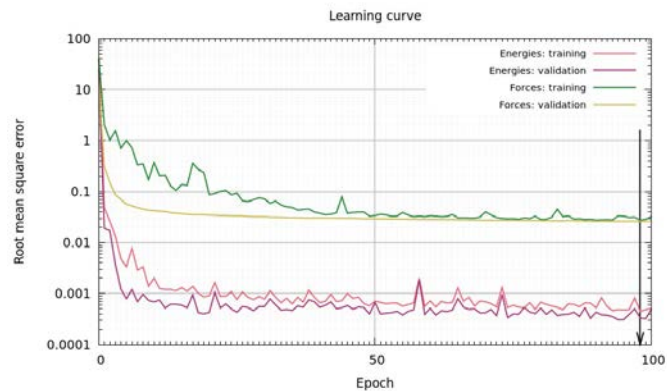
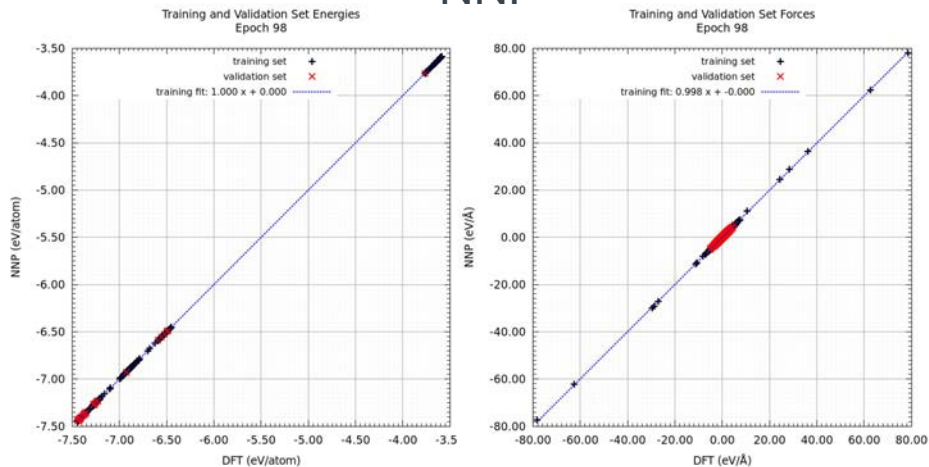
AlN (001) surface slab

Machine Learned Potential

SNAP



NNP



Elastic and Vibrational Properties

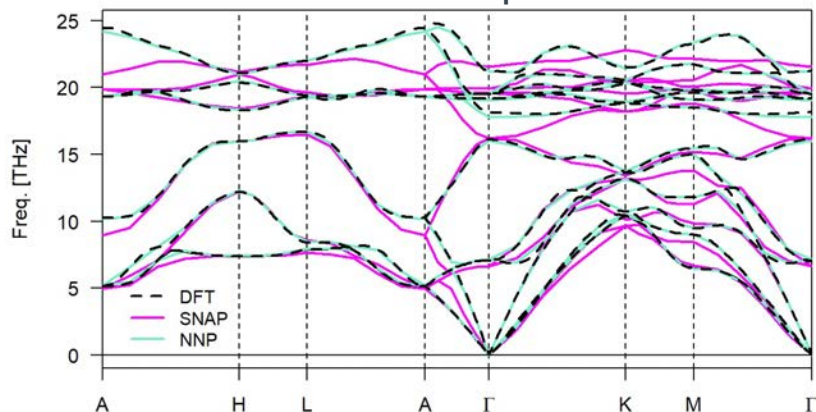
NNP

- Excellent phonon dispersion
- Good elastic properties

SNAP

- Good phonon dispersion
- Good elastic properties

Phonon dispersion



Elastic moduli (GPa)



[1] C.M. Lin et al., Appl. Phys. **109**, 033514 (2011) [2] McNeil et al., J. Am. Ceram. Soc. **76**, 1132 (1993)

Thermal Conductivity with Green-Kubo

- Green-Kubo expression relating lattice thermal conductivity to the integral of the time autocorrelation function of the heat-flux density

$$\kappa(t_m) = \frac{1}{\Omega k_B T^2} \int_0^{t_m} \langle J(t) \cdot J(0) \rangle dt$$

Ω volume, k_B Boltzmann constant, T temperature, J thermal current

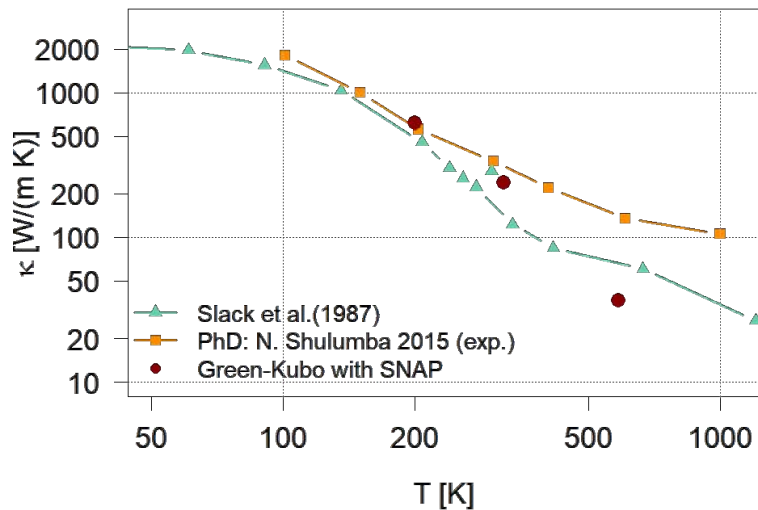
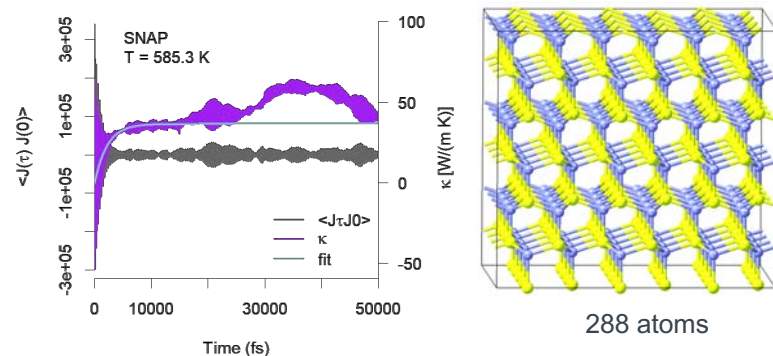
- Thermal current: $J(t) = \frac{d}{dt} \sum_i r_i(t) \epsilon_i(t)$

$r_i(t)$ time-dependent coordinate of atom i , $\epsilon_i(t)$ site energy

Temperature [K]	exp. κ [W/(mK)]	calc. κ [W/(mK)]
300	285 ^[1] , 320 ^[2]	238 (@320 K)

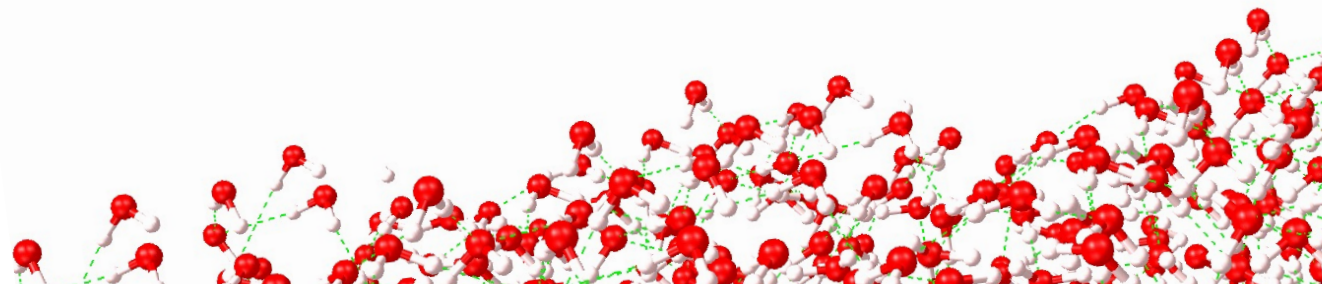
[1] G. A. Slack, R. Tanzilli, R. Pohl, and J. Vandersande, J. Phys. Chem. Solids **48**, 641-647 (1987)

[2] PhD: N. Shulumba, Linköping University (2015)

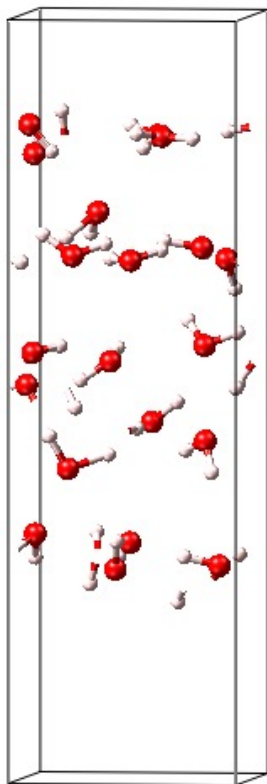


Water

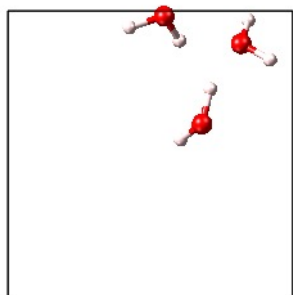
The Accuracy of MLPs



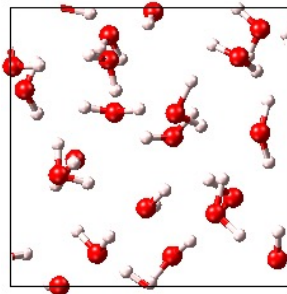
Training Set



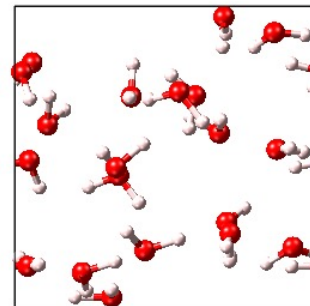
water slab



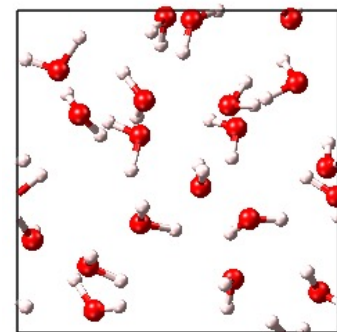
3 water molecules



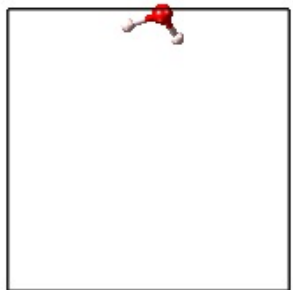
$\rho = 1100 \text{ kg/m}^3$



$\rho = 1000 \text{ kg/m}^3$



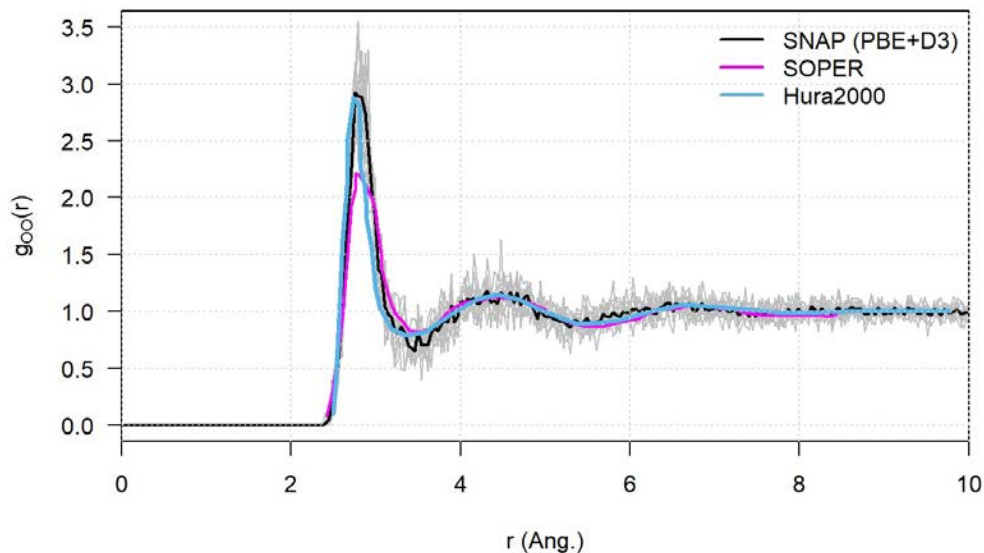
$\rho = 900 \text{ kg/m}^3$



1 water molecules

- Training set composed of VASP MD simulations
- VASP: PBE with van der Waals D3-zero-damping corrections

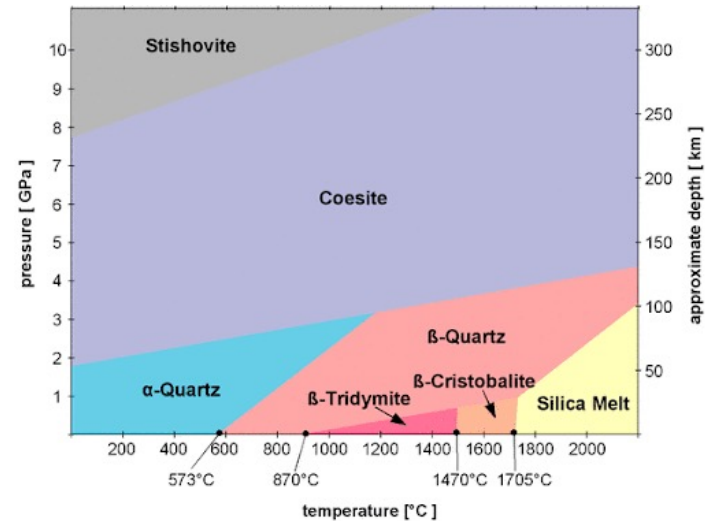
Water Structure



- Excellent $g_{00}(r)$ agreement with exp.
- Density (298.2K, 1atm): 991.6 kg/m³
exp.: 997 kg/m³
- H-O-H angle: 103.4° (4.3°)
exp.: 104.45°

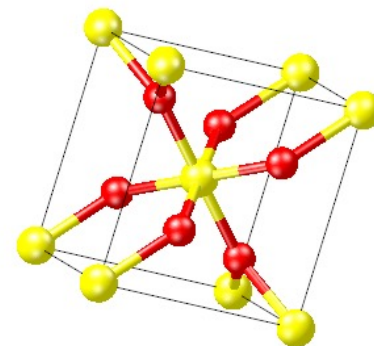
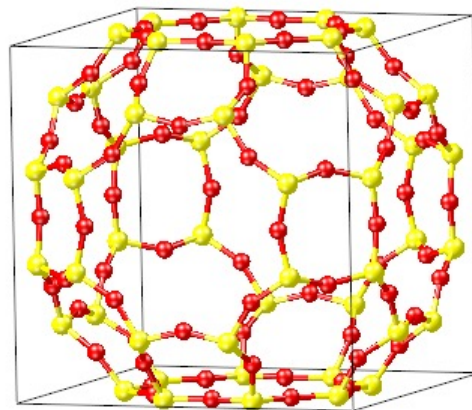
SiO₂ Polymorphs

A Single MLP for a Multitude of Structures

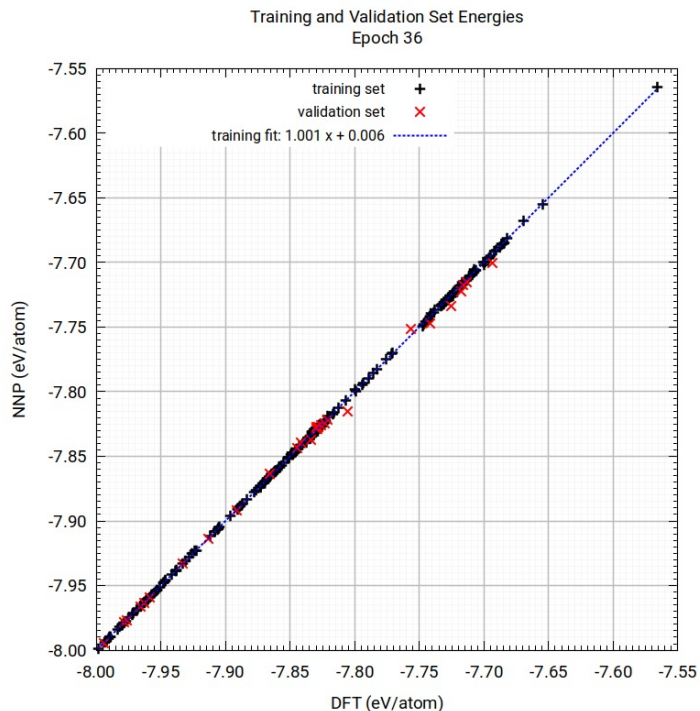


Structures and Data for Fit

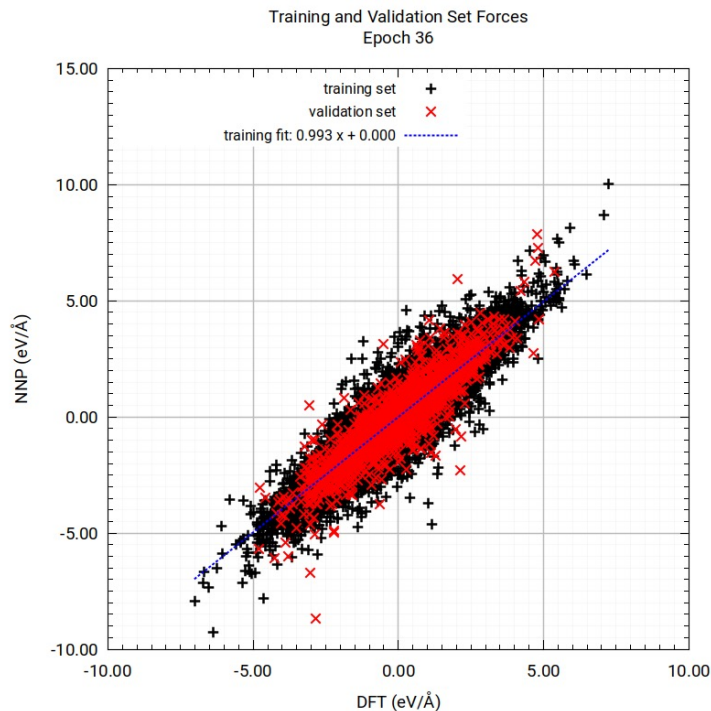
- Structures used to fit MLPs
 - α -quartz (2x2x2), zeolite Linde Type A, stishovite (2x2x2)
 - Cells distorted by -6%, -4%, -2%, 2%, 4%, 6% along a, b and c (simultaneous and separate), -4%, -2%, 2% and 4% for α , β and γ
 - NPT MD simulations at 298, 1100 and 1900 K for quartz and stishovite
 - Total of 298 structures
- VASP parameters
 - GGA-PBE with Grimme D3 correction
 - Plane wave cutoff 510 eV
 - k spacing 0.178
- SNAP and NNP fitted



Quality of Fit

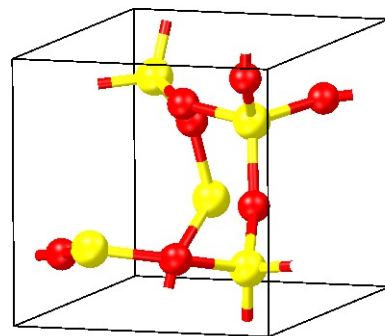
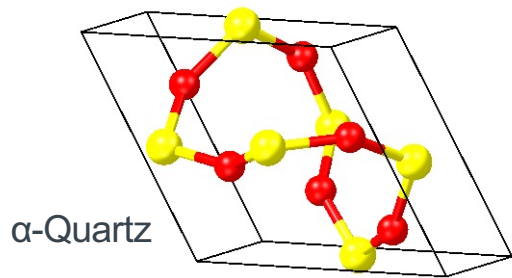


Energies



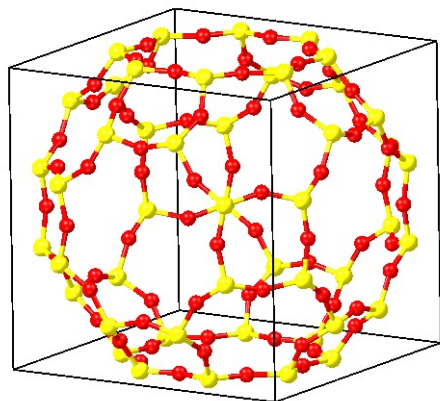
Forces

Validation of MLPs

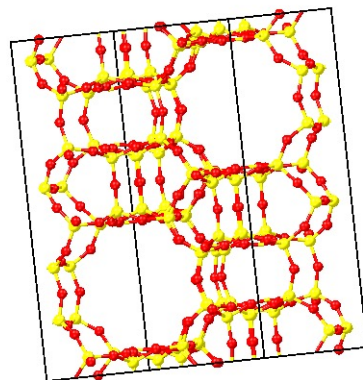


α -Cristobalite

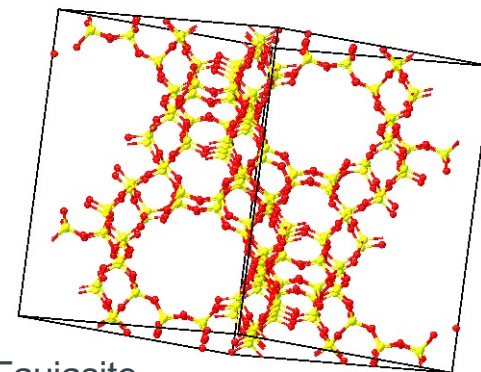
Stishovite



Linde type A

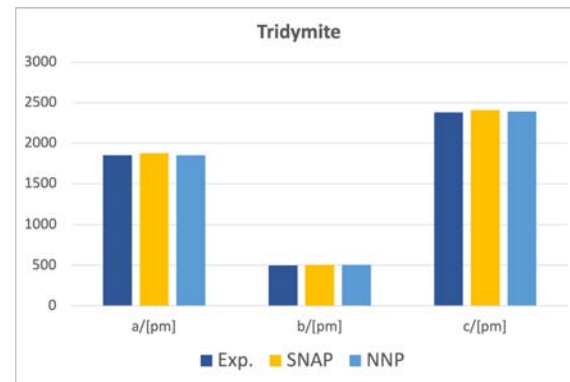
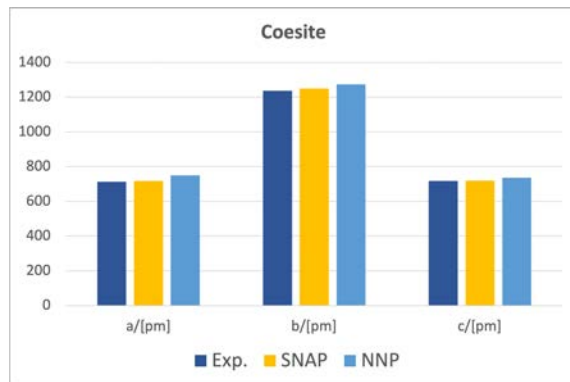
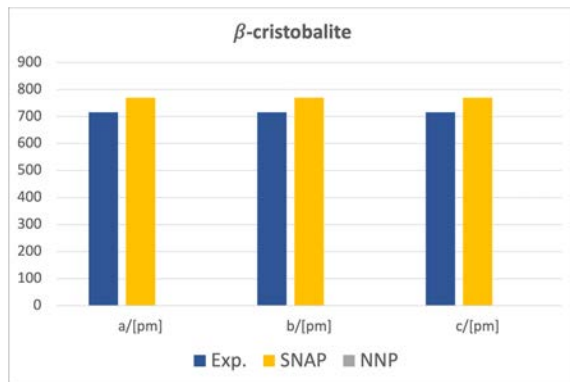
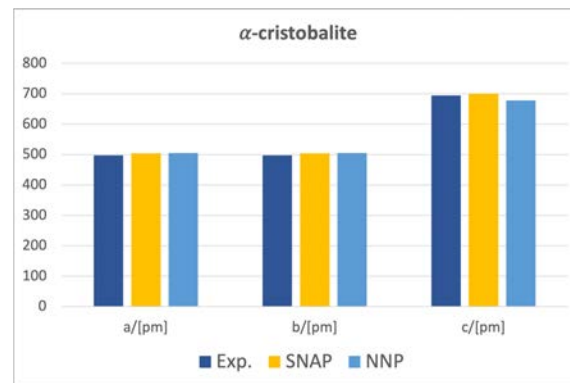
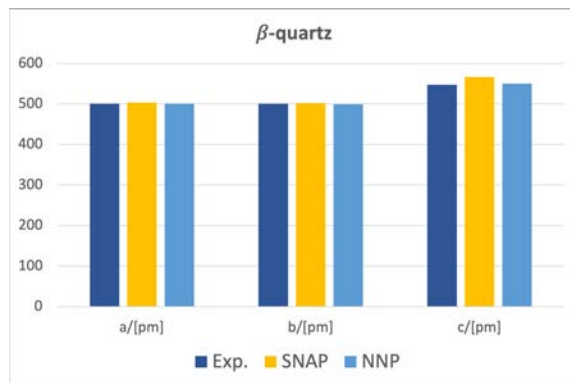
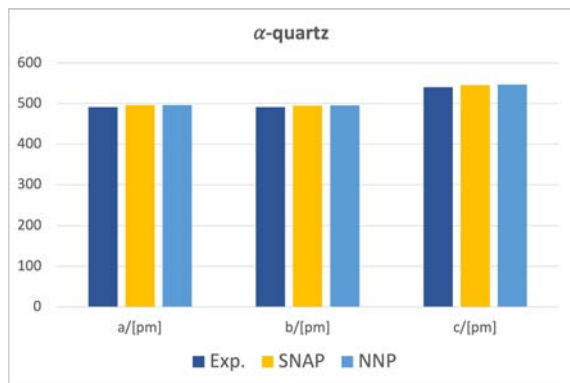


ZSM-5

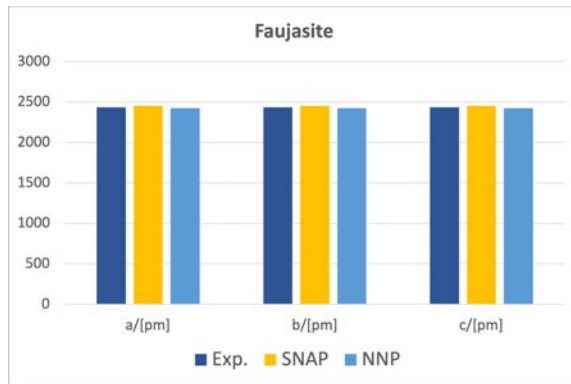
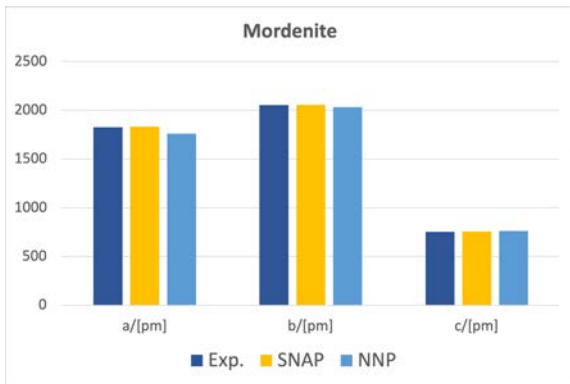
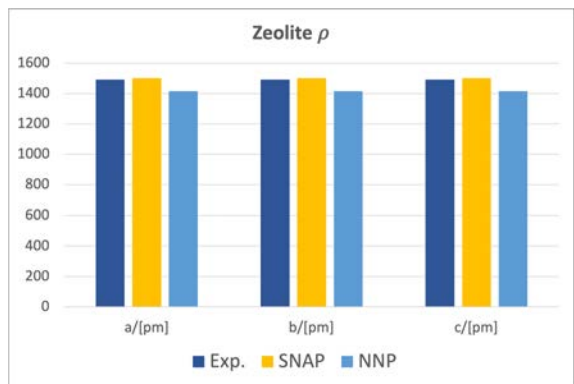
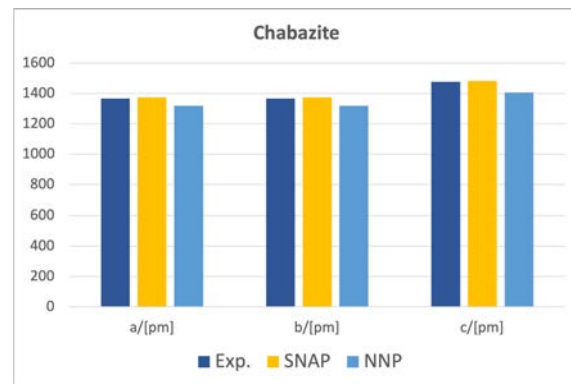
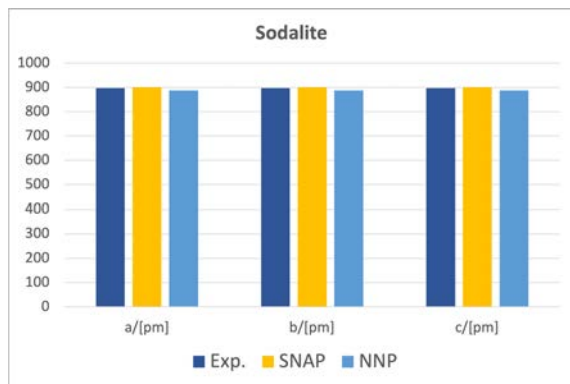
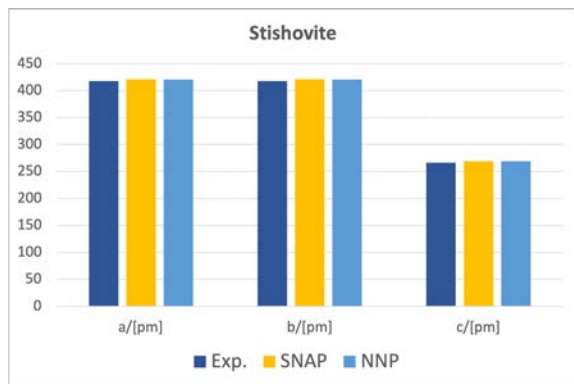


Faujasite

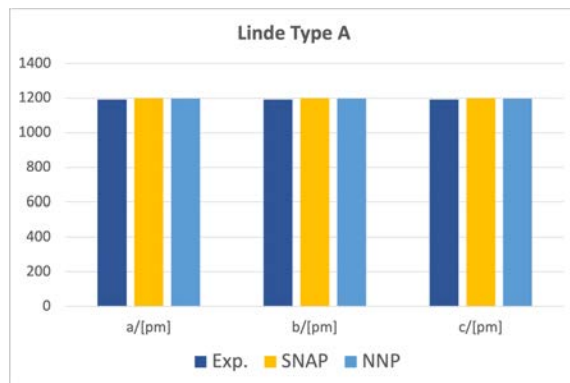
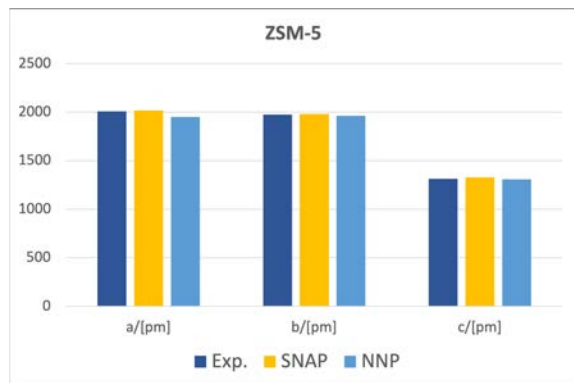
Results



Results

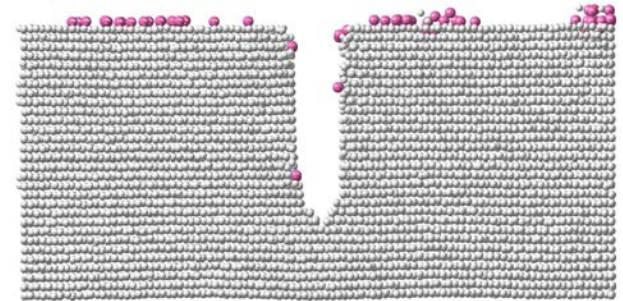
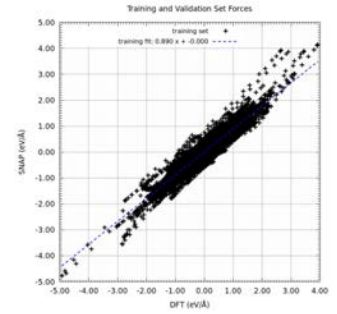


Results



Maximum deviation: 7.4 % (β -cristobalite), 5.1 % (coesite)

Iodine on Zr



Impact of Iodine Molecules on a Zirconium Surface with Nano-Groove

Generation of MLP: Training Set

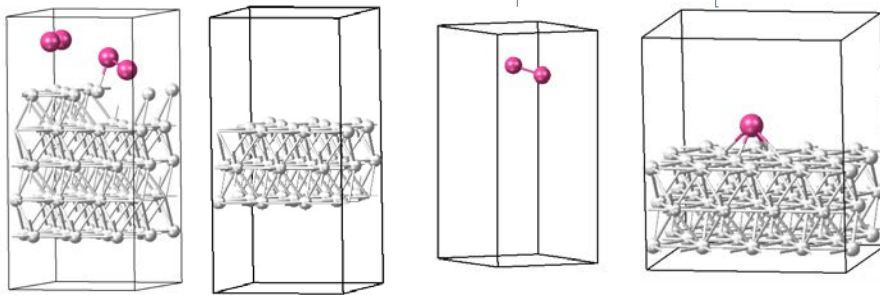
MedeA: structure list editor

File Add structure(s) Display Properties QT: QSAR Toolbox

SQLite structure list file (1011712 bytes): C:/Active/MLPG demo/Iodine on Zr/Zr-iodine-1.sli
Containing 4 structure(s)

Display structures from: to:

Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters
1	Iodine on Zr surface	Zr56I4	60	100	P1	9.70277 11.2038 20.90 90 90
2	Zr 3-layer slab	Zr36	36	100	P1	9.70277 11.2038 20.90 90 90
3	I2 molecule	I2	2	10	P1	9.70277 11.2038 20.90 90 90
4	Zr(0001) slab with I atom heating to 1500 K	Zr48I	49	100	P1	12.9989 11.2574 15.90 90 90



For each of these small structures, short *ab initio* molecular dynamics simulations were carried out using *MedeA* VASP, generating a total of 310 configurations. The energies, forces, and stress tensors are stored in a structure list.

Generation of SNAP with MLPG

Edit MLP generator stage 1

Training set: C:/Active/MLPG demo/Iodine on Zr/Zr-iodine-1.sli Select ...

Δ -learning: Fit potential Include potential

Δ -learning potential: Select ...

Type of machine learning potential: SNAP

Parameters for SNAP **Advanced**

Band limit: 8

Radial cutoff: 7.01456

Element	Relative radius	Weight	Energy shift
I	0.5	1.0	0.0
Zr	0.5	1.0	0.0

Fit: Energy Forces Stress

Weights: 1.0 0.01 1.0e-06

OK Cancel Help

Edit MLP generator stage 1

Training set: C:/Active/MLPG demo/Iodine on Zr/Zr-iodine-1.sli Select ...

Δ -learning: Fit potential Include potential

Δ -learning potential: Select ...

Type of machine learning potential: SNAP

Parameters for SNAP **Advanced**

Solver: SVD

Optimize: Radial cutoff Relative radii Weights

Use the Ziegler-Biersack-Littmark screened nuclear repulsion

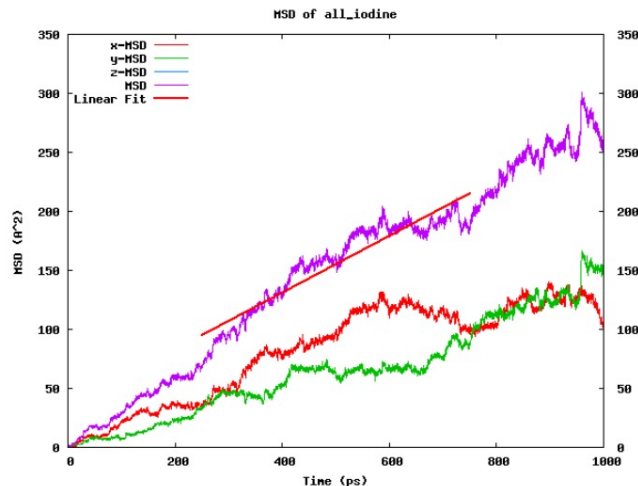
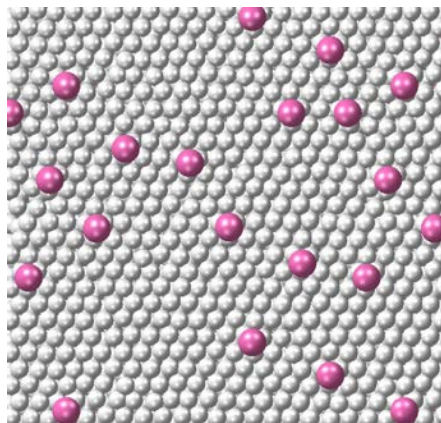
Inner cutoff: 0.5

Outer cutoff: 1.0

Include quadratic terms in energy model

OK Cancel Help

Diffusion of Iodine on Zr Surface



$$D = \frac{\langle R^2 \rangle}{\alpha t}$$

Mean-square displacement of per iodine atom vs. time during 1 ns with a time step of 1 fs (1 million configurations) using SNAP MLP on GPU. The model contains 1800 atoms.

Compute time: 3h 45 min (job T379)

T=1000 K

Quantity	Value	+/-	Uncertainty	Units
MSD D:	4.022e-06	+/-	1.9e-08	cm ² /s
MSD-X D:	7.762e-06	+/-	5.9e-08	cm ² /s
MSD-Y D:	4.302e-06	+/-	3.1e-08	cm ² /s
MSD-Z D:	1.13e-09	+/-	1e-10	cm ² /s



Concluding Remarks

MedeA MLP/MLPG

VASP accuracy with LAMMPS speed at your fingertips all within MedeA

- Machine-Learned-Potentials (MLPs) offer a combination of extended length and time scales with unprecedented ease in generation and high fidelity with respect to DFT to describe so far inaccessible physical phenomena.
- The MedeA MLP Generator (MLPG) offers a fully integrated workflow from training-set generation (using MedeA HT) and MLP generation to MLP application using MedeA LAMMPS.

MLPs with *MedeA LAMMPS*

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

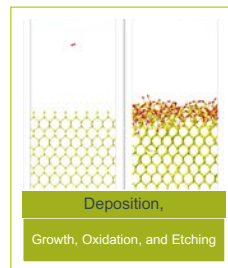
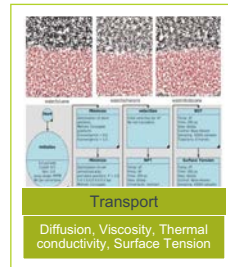
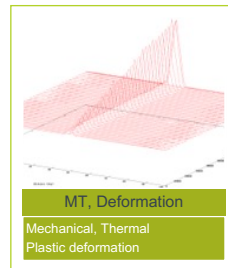
MedeA Viscosity: Calculate viscosity with Green-Kubo or non-equilibrium MD Müller-Plathe

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

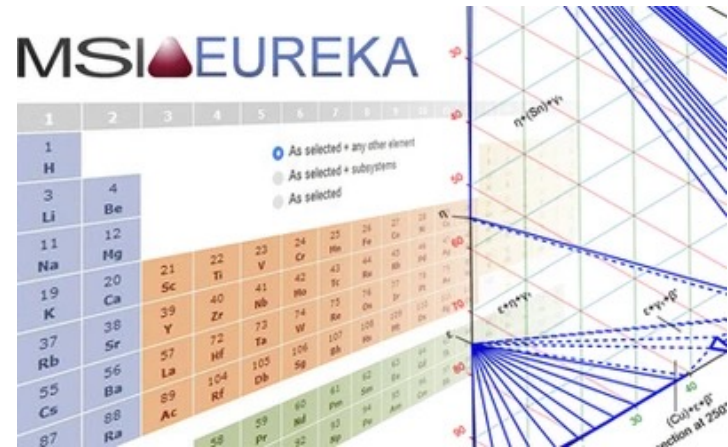
MedeA Phonon: Phonon spectra and thermodynamic functions (vibrational free energy, heat capacities)



Announcement

Upcoming

- Webinar Next Week: Materials Constitution Data in MSI Eureka – Fundamentals for Efficient R&D with Live Q&A
- The Medea 3.4 Release



Question and Answer Session



Dr. Erich Wimmer

Materials Design



Dr. Volker Eyert

Materials Design



Dr. David Reith

Materials Design

Questions about Materials Design Webinars

Katherine Hollingsworth

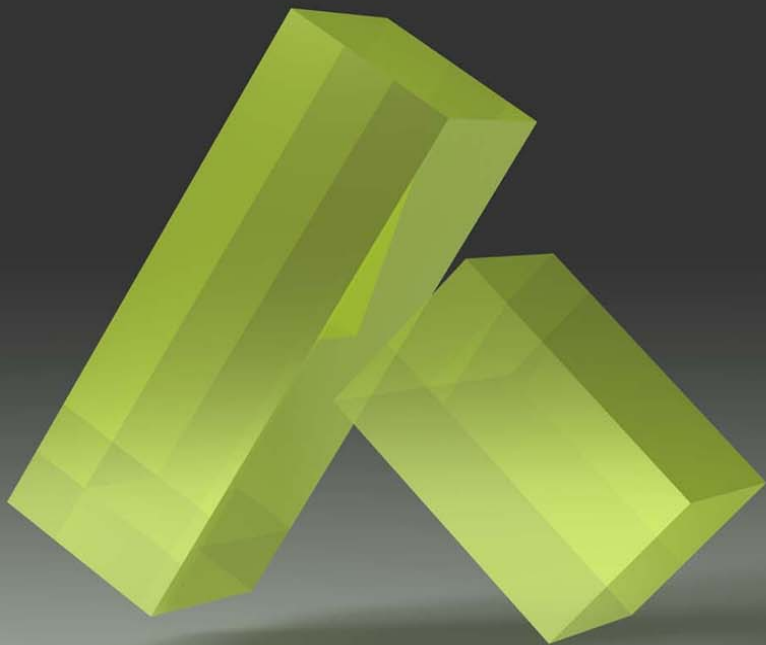
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MedeA

Innovation by Simulation