The OpenKIM Crystal Genome framework: high-throughput and portable evaluation of interatomic potentials for all known crystals

ilia Nikiforov

2025 LAMMPS Workshop and Symposium

Aug 13, Albuquerque, NM

University of Minnesota
Driven to Discover®

The OpenKIM Project (openkim.org)

OpenKIM is a curated repository of conventional and machine learning interatomic potentials that are compatible with many major simulation codes through a simple plug-and-play API. Each potential is verified for coding integrity and benchmarked against a variety of material properties, empowering users to discover and use the best potentials for their research. *Read more*

OpenKIM is funded by the NSF.

- Established 2009
- 661 interatomic models of many types
  - Classical (EAM, ReaxFF), ML (GAP, Nequip)
  - Largest repository of interatomic potentials on the web and growing!
  - OpenKIM content is contributed by OpenKIM staff and the community at large

The KIM API

- System-level package installable from conda, homebrew, or source
- Mature and stable
- Includes a package manager for downloading and installing potentials
- Let's say you want to use the following KIM potential in your simulation:
  `EAM_Dynamo_PunYamakovMishin_2015_NiCo__MO_010613863288_000`

```
$ conda install -c conda-forge kim-api lammps
$ kim-api-collections-management install user EAM_Dynamo_PunYamakovMishin_2015_NiCo__MO_010613863288_000
```

Use the potential in a LAMMPS simulation:

```
# Initialization
kim init EAM_Dynamo_PunYamakovMishin_2015_NiCo__MO_010613863288_000 metal

# System definition
read_data data.Co3Ni

# Potential setup
kim interactions Co Ni

# Run
run 0
```

https://docs.lammps.org/kim_commands.html

Analogous non-KIM input:

```
# Initialization
units metal

# System definition
read_data data.Co3Ni

# Potential setup
pair_style eam/alloy
pair_coeff * * Mishin_updated-Ni-Co-2013.eam.alloy Co Ni

# Run
run 0
```

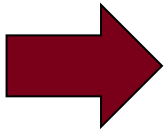
- Let's say you want to use this potential instead:
  `Sim_LAMMPS_HybridOverlay_BelandLuOsetskiy_2016_CoNi__SM_445377835613_001`
- This is also an EAM potential, but it's combined with ZBL short-range repulsion for high-energy collisions
- Install it:

```
$ kim-api-collections-management install user Sim_LAMMPS_HybridOverlay_BelandLuOsetskiy_2016_CoNi__SM_445377835613_001
```

If you use KIM, the only thing that changes is the model name:

```
# Initialization
kim init Sim_LAMMPS_HybridOverlay_BelandLuOsetskiy_2016_CoNi__SM_445377835613_001 metal

# System definition
read_data data.Co3Ni

# Potential setup
kim interactions Co Ni

# Run
run 0
```

```
# Initialization
units metal

# System definition
read_data data.Co3Ni

# Potential setup
pair_style eam/alloy
pair_coeff * * Mishin_updated-Ni-Co-2013.eam.alloy Co Ni

# Run
run 0
```



Analogous non-KIM input changes a lot!

```
# Initialization
units metal

# System definition
read_data data.Co3Ni

# Potential setup -- only works for
# atom types Co=1, Ni=2
pair_style hybrid/overlay zbl 0.5 2.0 eam/alloy
pair_coeff 1 1 zbl 28 28
pair_coeff 1 2 zbl 27 28
pair_coeff 2 2 zbl 27 27
pair_coeff * * eam/alloy NiCo-lammps-2014.alloy Co Ni

# Run
run 0
```

Other Simulation Software

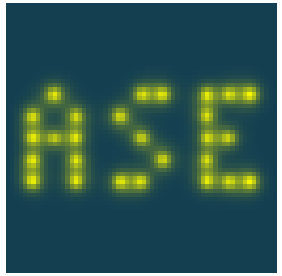
- Many other simulation codes besides LAMMPS support the KIM API with analogous model-type-agnostic plug-and-play support

GULP

Asap

Fit KIM-compliant ML and classical potentials!

DL_POLY



and more

KIM Processing Pipeline

OpenKIM is a curated repository of conventional and machine learning interatomic potentials that are compatible with many major simulation codes through a simple plug-and-play API. Each potential is verified for coding integrity and benchmarked against a variety of material properties, empowering users to discover and use the best potentials for their research. *Read more*

OpenKIM is funded by the NSF.

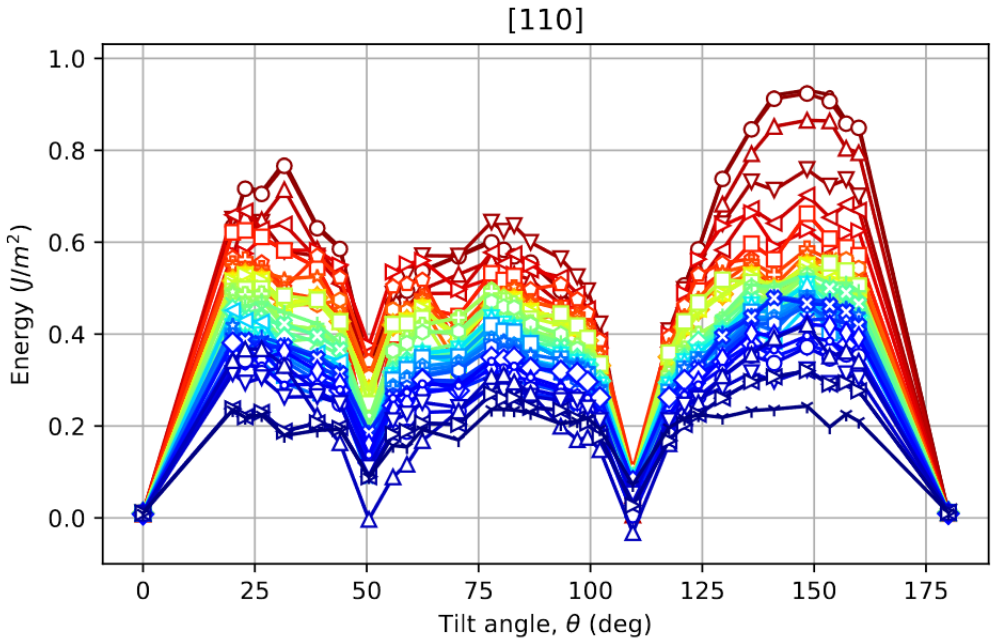
- Each potential that is uploaded to OpenKIM is automatically run through a host of computations using our distributed computational pipeline that sends computations to several HPCs around the country
- *Verification Checks:* rotation/translation invariance, PBC support, force/energy derivative correctness, continuity of energy and derivatives, memory leaks, thread safety…

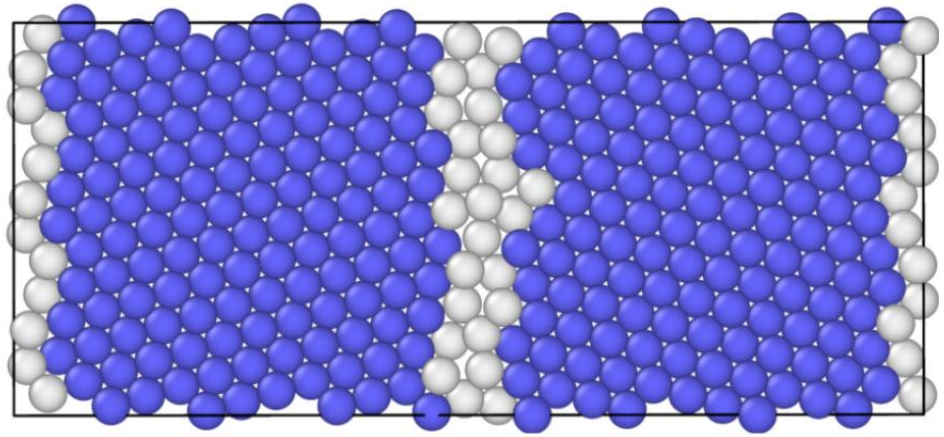
Karls *et al.* (2020), The OpenKIM processing pipeline: A cloud-based automatic material property computation engine. *J. Chem. Phys.* 153, 064104

OpenKIM property computations before Crystal Genome

- Lattice parameters
- Cohesive energy curves
- Elastic constants
- Surface energies
- Stacking fault energies
- Grain boundary energies
- Dislocation core energies
- Coefficient of thermal expansion
- Phonon dispersion relations and DOS
- Vacancy formation and migration properties

- Each computed for hundreds of IPs and queryable, enabling evaluation of IP accuracy, studies of correlations between material properties, and approximations of those properties outside the scope of DFT



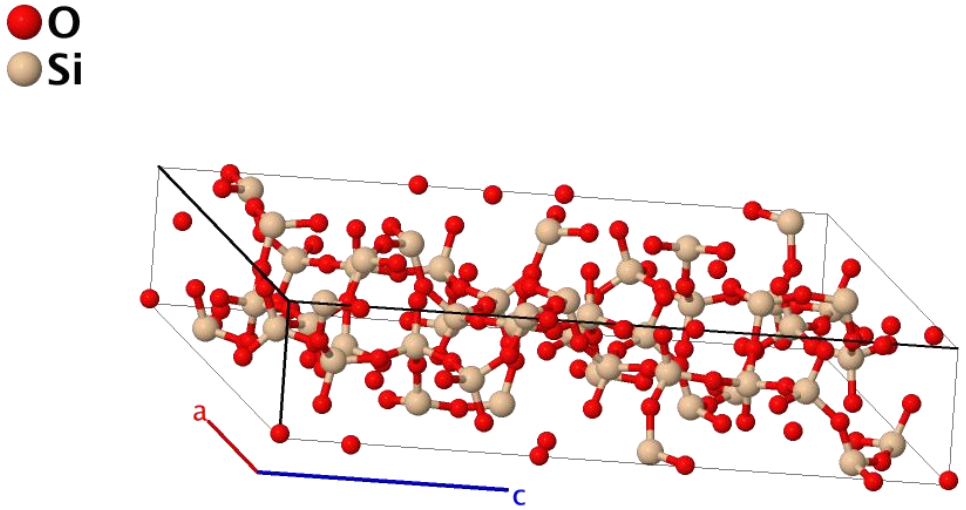


Waters *et al.* (2023). Automated determination of grain boundary energy and potential-dependence using the OpenKIM framework. *Computational Materials Science, 220, 112057.*

Before Crystal Genome, only for common single-element structures

- FCC, BCC, simple cubic, diamond, HCP…
  - Important and interesting, but only a tiny fraction of all possible crystals
  - Inorganic Crystal Structure Database (ICSD) contains 262,242 crystal structures

SiO_2 in the monoclinic low tridymite structure



$MgCuAl_2$ in the $E1_a$ structure

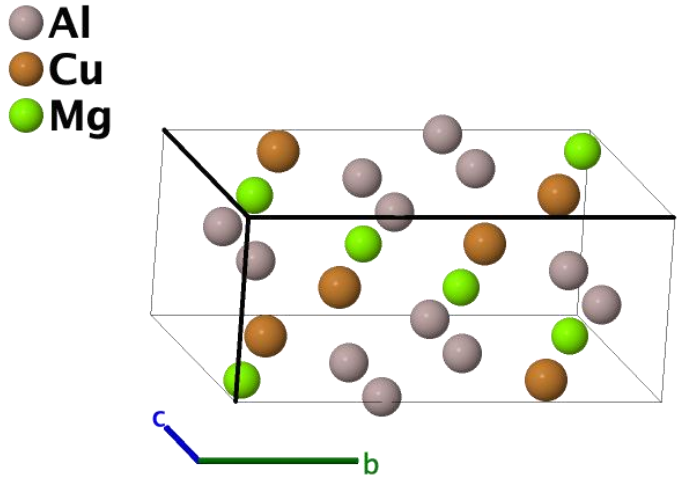
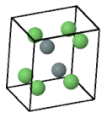


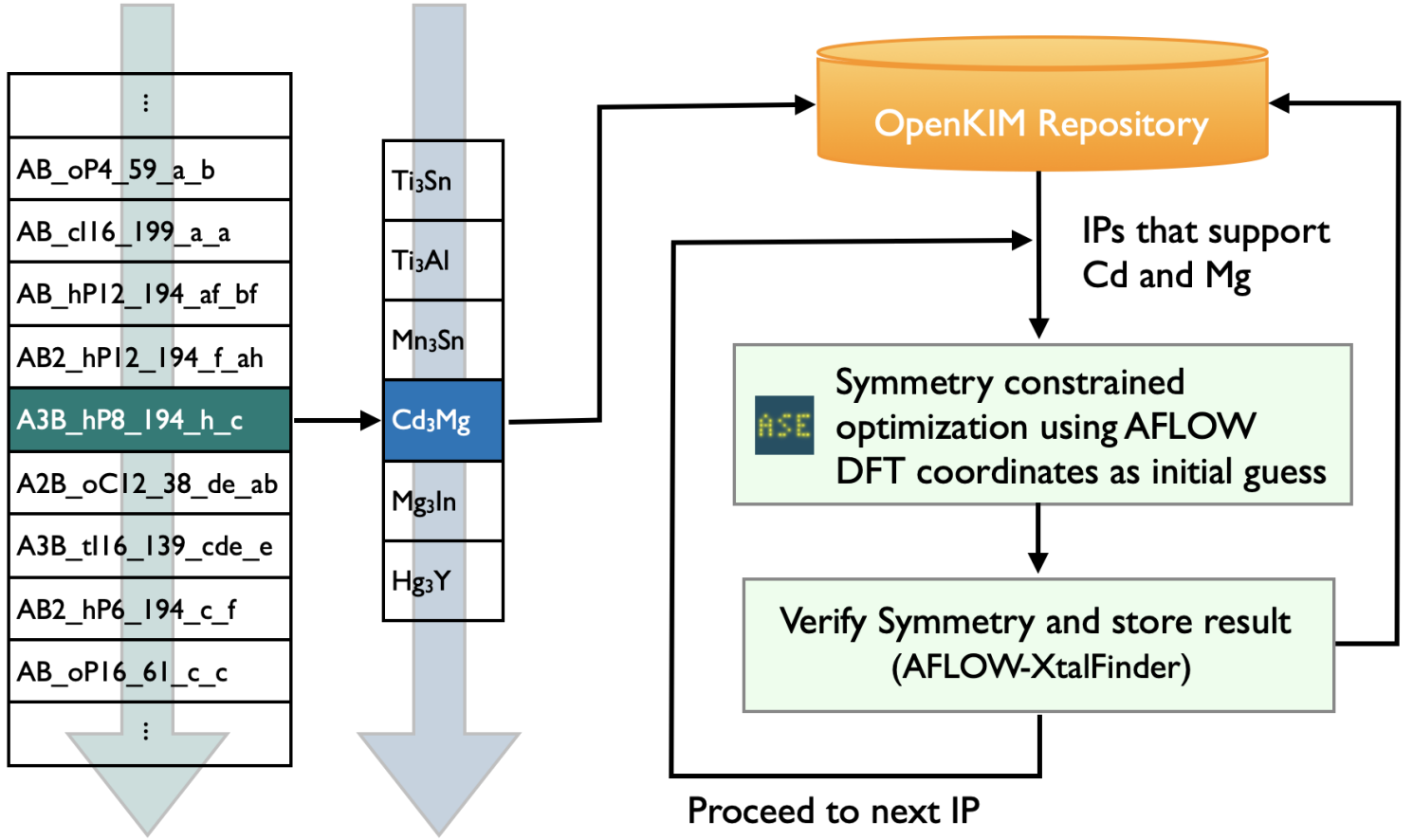
Image sources: AFLOW.org prototype library

Crystal Genome: property computations for arbitrary crystals

- Use the AFLOW prototype designation to classify materials (https://aflow.org/)
- So far, we have 32000+ unique crystals from the AFLOW DFT database
  - Provides reference data for evaluating IP performance
- For the first time, our protocols are easily accessible as part of the kimvv Python package (https://github.com/openkim/kimvv)
  - Can run with KIM Models
    - Which are possible to create locally from any LAMMPS pair_style
  - Or ASE Calculators
    - Theoretically even DFT! Have not tested, but DFTB works.



Schematic workflow for "Equilibrium Crystal Structure"



AFLOW
Automatic - FLOW for Materials Discovery

H. Eckert, *et al.* (2024). The aflow library of crystallographic prototypes: Part 4. *Computational Materials Science, 240:112988.*

The new OpenKIM front page

OpenKIM

Select species

Search for Predictions

Search for Potentials

Next slides

All IPs archived on OpenKIM have dedicated model pages with a wealth of metadata and predictions. In addition, for each IP, all papers citing the IP are listed with information on which actually used the IP in a simulation using the Deep Citation ML framework

EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005

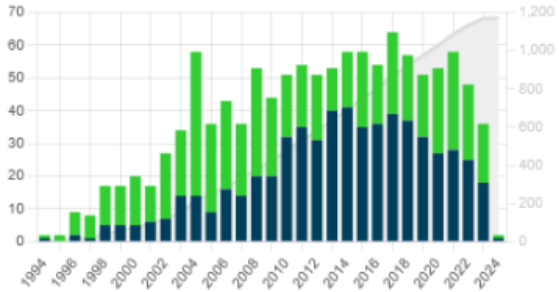
Interatomic potential for Aluminum (Al).

Use this Potential

Title	EAM potential (LAMMPS cubic hermite tabulation) for Al developed by Ercolessi and Adams (1994) v005

Citations

This panel provides information on past usage of this interatomic potential (IP) powered by the OpenKIM Deep Citation framework. The ***word cloud*** indicates typical applications of the potential. The ***bar chart*** shows citations per year of this IP (bars are divided into articles that used the IP (green) and those that did not (blue)). The ***complete list of articles*** that cited this IP is provided below along with the Deep Citation determination on usage. See the Deep Citation documentation for more information.



1171 Citations (575 used)

Show Model Used | Show All | Search here | Search | Clear | Sort By Usage

Help us to determine which of the papers that cite this potential actually used it to perform calculations. If you know, click the 💬.

USED (high confidence) V. Shenoy, "Multi-scale modeling strategies in materials science—The quasicontinuum method," *Bulletin of Materials Science*. 2003. link Times cited: 15

USED (high confidence) W. Cai, V. Bulatov, J. Chang, J. Li, and S. Yip, "Chapter 64 – Dislocation Core Effects on Mobility." 2004. link Times cited: 128

USED (high confidence) D. Olmsted, R. E. Phillips, and W. Curtin, "Modelling diffusion in crystals under high internal stress gradients," *Modelling and Simulation in Materials Science and Engineering*. 2004. link Times cited: 23

Abstract: Diffusion of vacancies and impurities in metals is important... read more

USED (high confidence) Al, M. Dewald, and W. Curtin, "Multiscale modelling of dislocation/grain-boundary interactions: I. Edge dislocations

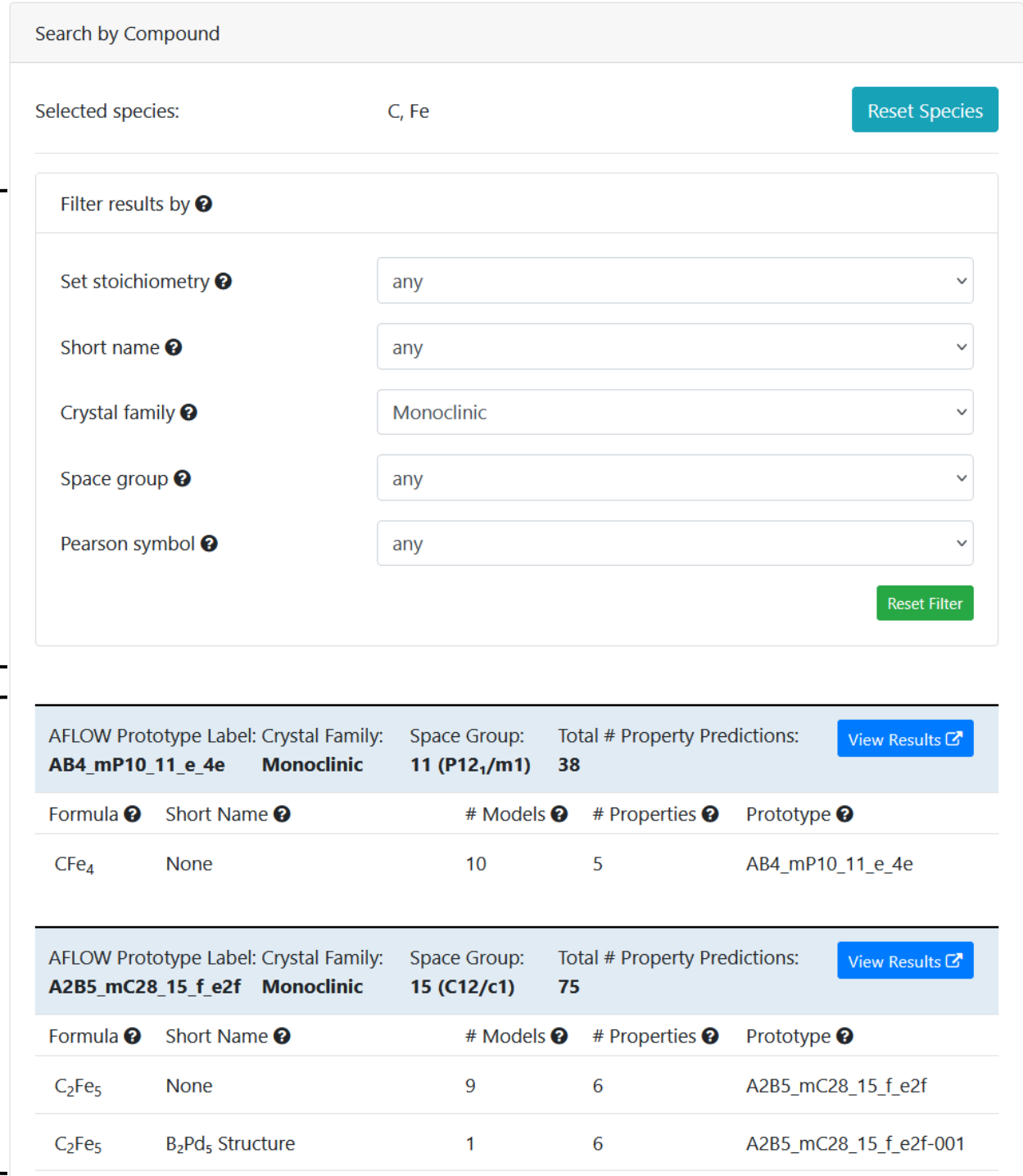
Description	This is an EAM parameterization for pure aluminum due to F. Ercolessi and J. B. Adams. The potential was developed using the "force-matching method", which includes forces from first-principles calculations in the fitting data base. The potential was fitted to properties of face-centered cubic (fcc) crystals.
Species	Al

Crystallography-based material search

Several filters for narrowing your search

Click on ? for explanations

Summary table for each unique crystal structure fitting the chosen criteria



Interatomic Potential Material Property Predictions

Prototype Label: A2B5_mC28_15_f_e2f + crystallography

Chemical Formula: C_2Fe_5

Results for: MEAM_LAMMPS_Lee_2006_FeC__MO_856956178669_002 Interatomic Potential page

2 unique initial structures found for this prototype label and potential MEAM_LAMMPS_Lee_2006_FeC__MO_856956178669_002
12 property predictions

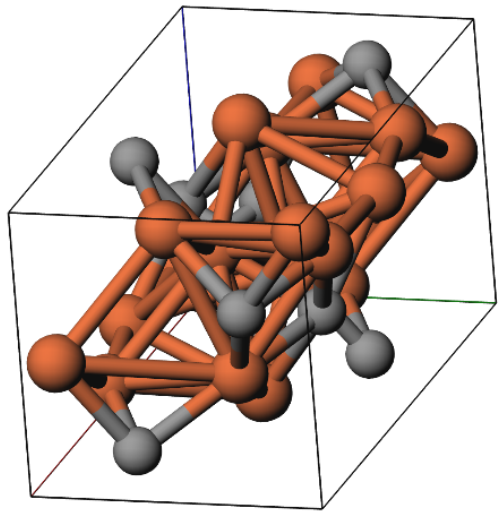
Select interatomic potential to view predictions

× Structure A

Zero temperature and stress equilibrium structure

Structure Prototype Label: A2B5_mC28_15_f_e2f + crystallography

Short Name: None



High-quality views
Unit cell | 2 x 2 x 2 supercell | 20Å box

Annotated views
Unit cell | 2 x 2 x 2 supercell | 20Å box

Orientation
a | b | c
x | y | z
Trimetric (default)
Zoom In | Zoom Out | Zoom 100%

Animation
Pitch | Yaw | Roll | Tumble | Pause

Link to POSCAR File
Right click on structure to view menu

Crystallography and visualization

+ Equilibrium crystal structure at a given temperature and stress state
+ Energy and crystal structure as a function of hydrostatic pressure for an arbitrary crystal
+ Equilibrium crystal structure and binding potential energy at zero temperature and applied stress
+ Isothermal bulk modulus of a crystal at a given temperature and stress state
+ Isothermal elastic constants of a crystal at a given temperature and stress state
+ Mass density of a crystal at a given temperature and stress state

Computed properties
Coming soon:
- Vacancies
- Phonons
- Heat capacity
- Free energy
- Anisotropic thermal expansion

Equilibrium crystal structure at a given temperature and stress state

Equilibrium crystal structure at a given temperature and stress state
(For more information, see the property definition crystal-structure-npt)

Lattice constant *a* (angstrom): 11.234929928428233

Other crystal structure parameters:

b/a	0.42472470666329754
c/a	0.4468002986883784
beta	80.90760525070152
y1	0.5544700195200984
x2	0.6171745239144182
y2	0.19748804597590167
z2	0.9111239776967639
x3	0.09458982196358723
y3	0.9385674623523419
z3	0.5964733752698224
x4	0.7161864807937353
y4	0.8915113310132552
z4	0.6992855777017595

Cauchy Stress (eV/angstrom^3):

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Temperature (K): 0.0

Developer Mode

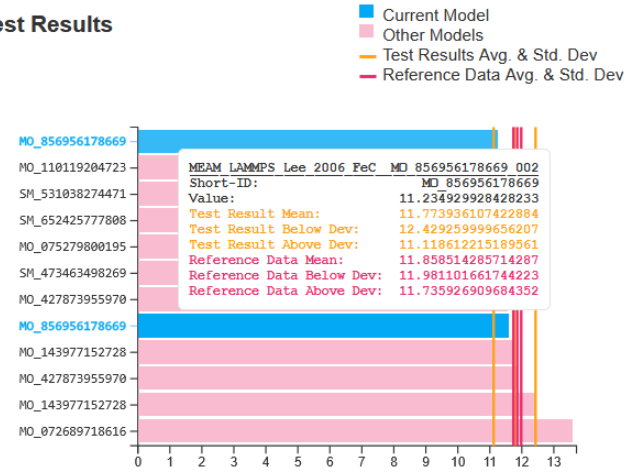
OpenKIM

Property: crystal-structure-npt
Species: C,Fe
Prototype Label: A2B5_mC28_15_f_e2f

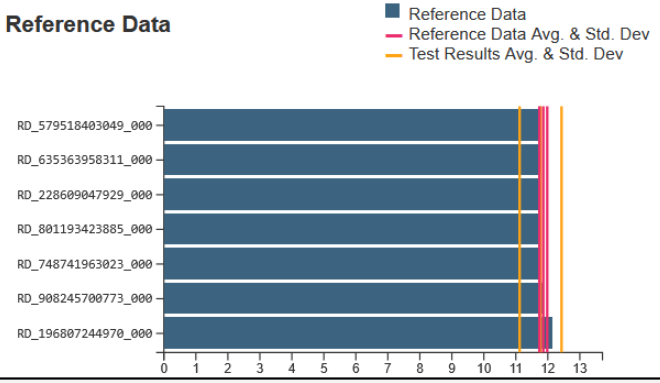
Data to plot: a (angstrom)

Display: Model Average & SD, Reference Data Average & SD

Test Results



Reference Data

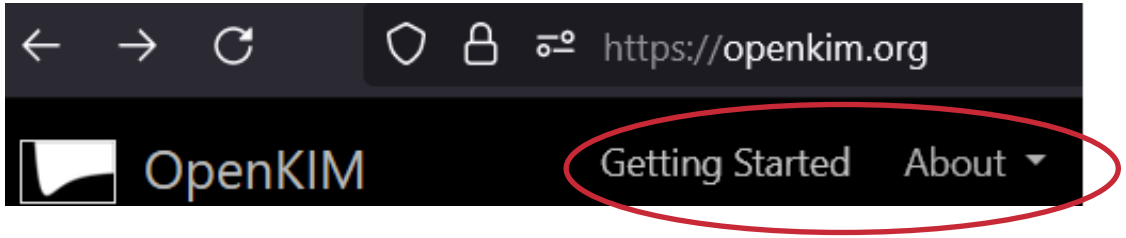


View figure in

- Property summary
  - Symmetry-reduced when possible, e.g.
    - Symmetry-reduced coordinates and lattice parameters
    - Unique elastic constants
  - Click on ? for explanations of each field
- Interactive bar chart comparing with other models and reference data when available

Where to get more info

- Breakout session tomorrow with an intro to crystallography, website tour, and example local computations



- support@openkim.org
- MatSci.org – discussion forum coordinated by OpenKIM and Materials Project, nearly 40 participating projects incl. LAMMPS
- kim-initiative.org – KIM is part of an initiative of interrelated projects, including several exciting ML projects for fitting MLIPs and material generation

MATSCI COMMUNITY DISCOURSE

Thank you!

- To the organizers and the audience
- To all the past and present OpenKIM team members and contributors: https://openkim.org/about/#team-members