

TUTORIAL: The OpenKIM.org repository, property testing framework, and KIM models

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4/22/2023

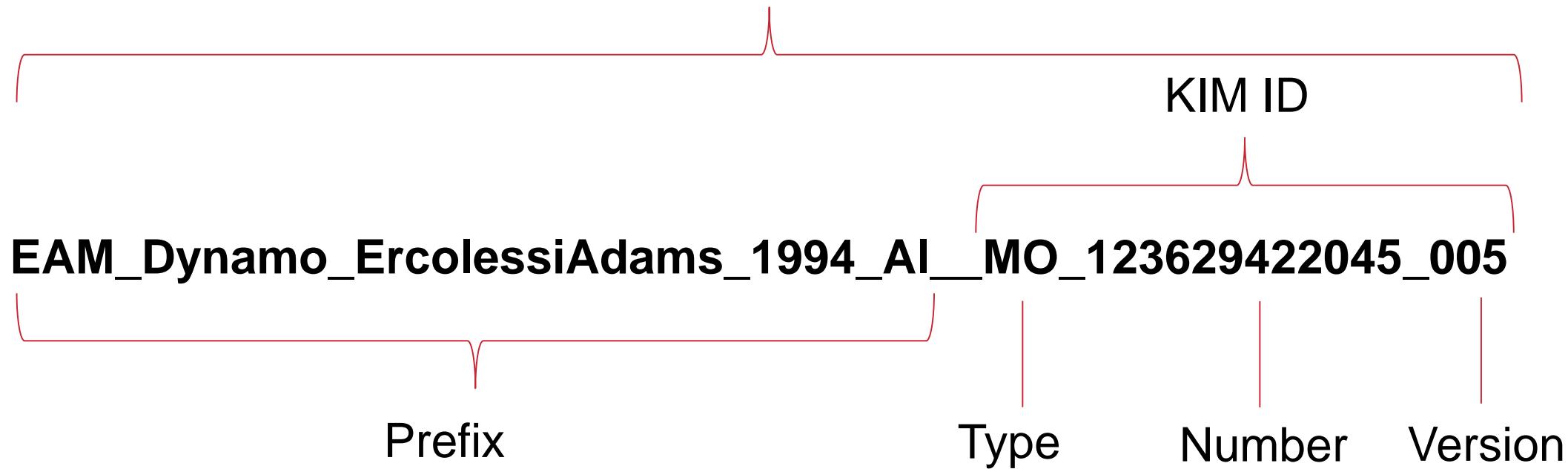


Hands-on tutorial

- Binder repo:
 - <https://github.com/openkim/openkim-demo>
 - Click the “launch binder” icon: A rectangular button with a dark grey background and a light blue right side. It features a small circular icon with a white 'b' inside on the left, followed by the words 'launch' and 'binder' in white.
 - The repo also contains a PDF of these slides

KIM IDs:

Extended KIM ID



<https://openkim.org/doc/schema/kim-ids/>



OpenKIM content: Models

- *Models*: interatomic potentials
 - Portable models (“MO”):
 - Self-contained, can work through the KIM API with any compatible *simulator* (term for simulation code)
 - May or use a *Model Driver* (“MD”):
 - In this case, the *model* encapsulates the parameters, and the *model driver* contains the code to compute forces and energies
 - Simulator models (“SM”):
 - Works only with a specific *simulator*. Currently only LAMMPS (and by extension ASE through the lammpslib and lammpsrun interface)
 - Within LAMMPS and ASE, works exactly like any other KIM model



OpenKIM content: *Tests*

- *Tests* (“TE”) are programs that automatically pair with *models* to compute their predictions for material properties
 - These predictions take the form of *Property Instances* which are realizations of *Property Definitions* (a standardized format for reporting a material property)
 - May use a *Test Driver* (“TD”) executable, in which case the *test* encapsulates testing parameters such as species and crystal structure

<https://openkim.org/doc/schema/properties-framework/>



Other OpenKIM content

- *Reference Data* (“RD”):
 - Archived *property instances* from external sources (e.g. DFT computations)
- *Verification Checks* (“VC”):
 - “Tests” for coding integrity (objectivity, forces match numerical derivative of energy, memory leaks, etc).



Website demo slides



Access help,
browse content,
join as member (no
spam!)

Welcome to the Open Knowledgebase of Interatomic Models!

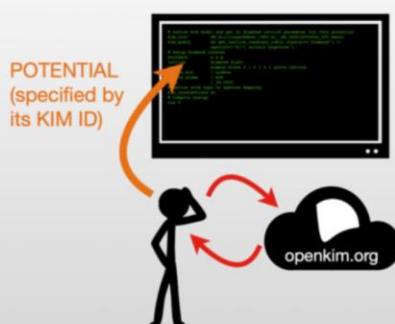
Potentials and analytics for making classical molecular simulations of materials
OpenKIM is open source and freely available. [Read more](#)

Image of a twisted graphene bilayer generated by Moon-ki Choi, University of Minnesota

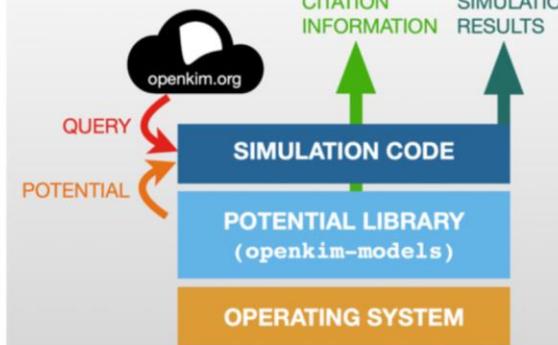
- 1** Install the OpenKIM Library of interatomic potentials (just once)



- 2** Write simulation input script with a potential selected by user on openkim.org



- 3** Run simulation using KIM potential and potential-specific material property queries



```
# Define KIM model and get Si diamond lattice parameter for this potential
kim_init      SW_StillingerWeber_1985_Si_MO_405512056662_005 metal
kim_query     a0 get_lattice_constant_cubic crystal=["diamond"] species=["Si"] u
# Setup diamond crystal
boundary      P P P
lattice       diamond ${a0}
region        simbox block 0 1 0 1 0 1 units lattice
create_box    1 simbox
create_atoms   1 box
mass          1 28.0855
# Define atom type to species mapping
kim_interactions Si
# Compute energy
run 0
```

[LAMMPS](#) | [ASE](#) | [DLPOLY](#) | [GULP](#) More examples.

Models

~~Click on an element to find it~~

H	Sp
Li	Be
Na	Mg
K	Ca
Rb	Sr
Cs	Ba
Fr	Ra

Browse Models and Tests by element

els that su

Submit a model to be added

Aluminum (Al)		N	O	F	He
Models: 54					Ne
Al	Si	P	S	Cl	Ar
Ga	Ge	As	Se	Br	Kr
In	Sn	Sb	Te	I	Xe
Tl	Pb	Bi	Po	At	Rn
Nh	Fl	Mc	Lv	Ts	Og

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Reliability

Content curated on OpenKIM comes from trusted sources and is reviewed by the [KIM Editor](#) for quality control. Each interatomic potential ("KIM Model") is subjected to a set of [Verification Checks](#) to ensure correct implementation and to provide diagnostic information on its performance. The predictions of each potential for a host of material properties are obtained through reliable computational protocols called [KIM Tests](#). All results are conveniently displayed on "Model Pages" accessible through the [OpenKIM browse interface](#). [Read more...](#)

Reproducibility

Each interatomic potential in openkim.org is associated with a unique KIM ID that identifies the potential and its version. In addition, each potential is issued a DOI that can be cited in publications. Since openkim.org archives the potential implementation (computer code), not just its parameters, this ensures the ability to reproduce results. All citation information is available in convenient form on the potential's Model Page, and is output by supported simulation codes. [Read more...](#)

Accessibility

Interatomic potentials in openkim.org are freely available and can be used directly with many [major molecular simulation packages](#) that conform to the [KIM API](#) simply by specifying their KIM IDs in the simulator input script (see code examples at top of page). The KIM infrastructure and library of potentials can be installed from binary through [most popular package managers](#) or from [source](#). A potential's predictions for material properties are accessible programmatically via RESTful [KIM web queries](#) and from within supported codes. [Read more...](#)

 News

05-Mar-2023

Agenda for the KIM Symposium at the 2023 Mach Conference is now available

The agenda is now available for the Symposium on "Systems for Fitting, Uncertainty Quantification, Selection and Use of Interatomic Models" orgaized by OpenKIM at the Mach Conference in Baltimore, MD on April 5-7, 2023.

22-Nov-2022

<https://openkim.org/browse/models/by-species?species-search=A>

Metrics

Model Drivers

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Models - by Species

Alphabetical By Species By Type By Driver By Tests By Developer

Models in the OpenKIM Repository

Each "model" is a specific parameterization of an interatomic model class for a given material system (e.g. the Lennard-Jones potential for Ar). [Click for more information.](#)

Choose from the tab above to sort the models in different ways.

When sorting by species, you can narrow the selection to find potentials th

Multiple ways to sort/categorize

Narrow species selection:

x Al Ti

Ti

Al

Browse all types of KIM content

Model	Simulator	Title
EAM_CubicNaturalSpline_ErcolessiAdams_1994_Al_MO_800509458712_002	Any	EAM potential (cubic natural spline tabulation) for Al developed by Ercolessi and Adams (1994) v002
EAM_Dynamo_AngeloMoodyBaskes_1995_NiAlH_MO_418978237058_005	Any	EAM potential (LAMMPS cubic hermite tabulation) for the Ni-Al-H system developed by Angelo, Moody and Baskes (1995) v005
EAM_Dynamo_CaiYe_1996_AlCu_MO_942551040047_005	Any	EAM potential (LAMMPS cubic hermite tabulation) for the Al-Cu system developed by Cai and Ye (1996) v005
EAM_Dynamo_ErcolessiAdams_1994_Al_MO_123629422045_005	Any	EAM potential (LAMMPS cubic hermite tabulation) for Al developed by Ercolessi and Adams (1994) v005
EAM_Dynamo_FarkasCaro_2020_FeNiCrCoAl_MO_820335782779_000	Any	EAM potential (LAMMPS cubic hermite tabulation) for the Fe-Ni-Cr-Co-Al system developed by Farkas and Caro (2020) v000
EAM_Dynamo_FarkasJones_1996_NbTiAl_MO_042691367780_000	Any	EAM potential (LAMMPS cubic hermite tabulation) for the Nb-Ti-Al system developed by Farkas and Jones (1996) v000
EAM_Dynamo_JacobsenNorskovPuska_1987_Al_MO_411692133366_000	Any	EMT potential (LAMMPS cubic hermite tabulation) for Al developed by Jacobsen, Norskov, and Puska (1987) v000
EAM_Dynamo_LandaWynblattSiegel_2000_AlPb_MO_699137396381_005	Any	Glue potential (LAMMPS cubic hermite tabulation) for the Al-Pb system developed by Landa et al. (2000) v005
EAM_Dynamo_LiuAdams_1998_AlMg_MO_019873715786_000	Any	EAM potential (LAMMPS cubic hermite tabulation) for the Al-Mg system developed by Liu and Adams (1998) v000
EAM_Dynamo_LiuErcolessiAdams_2004_Al_MO_051157671505_000	Any	EAM potential (LAMMPS cubic hermite tabulation) for Al developed by Liu, Ercolessi and Adams (2004) v000
EAM_Dynamo_LiuLiuBorucki_1999_AlCu_MO_020851069572_000	Any	EAM potential (LAMMPS cubic hermite tabulation) for the Al-Cu system developed by Liu et al. (1999) v000
EAM_Dynamo_LiuOhotnickýAdams_1997_AlMg_MO_559870613549_000	Any	EAM potential (LAMMPS cubic hermite tabulation) for the Al-Mg system developed by Liu et al. (1997) v000
EAM_Dynamo_MendelevAstaRahman_2009_AlMg_MO_658278549784_005	Any	Finnis-Sinclair potential (LAMMPS cubic hermite tabulation) for solid-liquid interfaces in Al-Mg alloys developed by Mendelev et al. (2009) v005
EAM_Dynamo_MendelevFangYe_2015_AlSm_MO_338600200739_000	Any	Finnis-Sinclair potential (LAMMPS cubic hermite tabulation) for the Al-Sm system developed by Mendelev et al. (2015) v000
EAM_Dynamo_MendelevFangYe_2008_Al_MO_338600200739_005	Any	Finnis-Sinclair potential (LAMMPS cubic hermite tabulation) for Al developed by Mendelev et al. (2008) v005

Multi-species selection



EAM_Dynamo_ZopeMishin_2003_TiAl_MO_117656786760_005

Interatomic potential for Aluminum (Al), Titanium (Ti).

[Use this Potential](#)

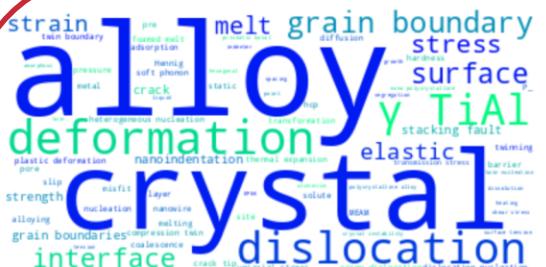
Quick navigation

Title ?

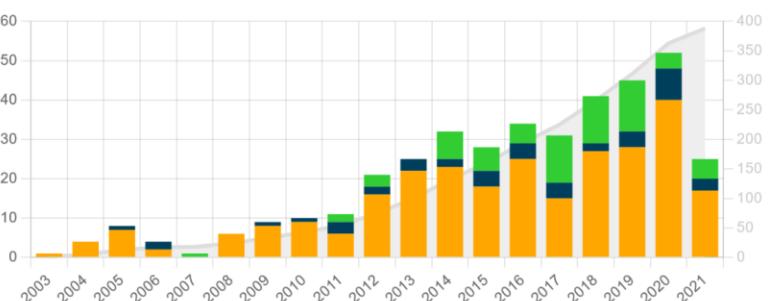
EAM potential (LAMMPS cubic hermite tabulation) for the Ti-Al system developed by Zope and Mishin (2003) v000

Citations ?

The word cloud indicates applications of this Potential. The bar chart shows citations per year of this Potential.



388 Citations (70 used)



★ Show Model Used Show All

Search here

Search

Clear

Sort By Newest

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

? Q. Pei, M. Jhon, S. Quek, and Z. Wu, "A systematic study of interatomic potentials for mechanical behaviours of Ti-Al alloys," *Computational Materials Science*. 2021. [link](#) Times cited: 1

Abstract: Intermetallic Ti-Al alloys exhibit attractive physical and m... [read more](#)

0 O. Ouadah, "Titanium Aluminide Coating: Structural and Elastic Properties by DFT Approach." 2021. [link](#) Times cited: 0

Abstract: The stability, elastic and electronic properties of titanium... [read more](#)

0 J. S. Smith et al., "Automated discovery of a robust interatomic potential for aluminum," *Nature Communications*. 2021. [link](#) Times cited: 5

Abstract: Machine learning, trained on quantum mechanics (QM) calculat... [read more](#)

? B. Bertin, J. Durinck, J. Grilhé, and J. Colin, "Grain boundary-induced plasticity during thin film buckling," *Mechanics of Materials*. 2021. [link](#) Times cited: 0

Description ?

EAM potential for Al, α -Ti, and γ -TiAl developed by fitting to a large database of experimental and ab initio data. The ab initio calculations were performed by the linearized augmented plane wave (LAPW) method within the density functional theory to obtain the equations of state for a number of crystal structures of the Ti-Al system. Some of the calculated LAPW energies were used for fitting the potentials while others for examining their quality. The potentials correctly predict the equilibrium crystal structures of the phases and accurately reproduce their basic lattice properties. The potentials are applied to calculate the energies of point defects, surfaces, and planar faults in the equilibrium structures. Unlike earlier EAM potentials for the Ti-Al system, the proposed potentials provide a reasonable description of the lattice thermal expansion, demonstrating their usefulness for molecular-dynamics and Monte Carlo simulations at high temperatures. The energy along the tetragonal deformation path (Bain transformation) in γ -TiAl calculated with the EAM potential is in fairly good agreement with LAPW calculations. Equilibrium point defect concentrations in γ -TiAl are studied using the EAM potential. It is



Citation info
(incl. ML-based
categorization of
type of usage)

Driver	EAM_Dynamo_MD_120291908751_005
KIM API Version	2.0
Potential Type	eam
Previous Version	EAM_Dynamo_ZopeMishin_2003_TiAl_MO_117656786760_004

Model Driver

VERIFICATION CHECK DASHBOARD

(Click here to learn more about Verification Checks)

Grade	Name	Category	Brief Description	Full Results	Aux File(s)
P ?	vc-species-supported-as-stated	mandatory	The model supports all species it claims to support; see full description .	Results	Files
P ?	vc-periodicity-support	mandatory	Periodic boundary conditions are handled correctly; see full description .	Results	Files
P ?	vc-permutation-symmetry	mandatory	Total energy and forces are unchanged when swapping atoms of the same species; see full description .	Results	Files
B ?	vc-forces-numerical-derivative	consistency	Forces computed by the model agree with numerical derivatives of the energy; see full description .	Results	Files
P ?	vc-dimer-continuity-c1	informational	The energy versus separation relation of a pair of atoms is C1 continuous (i.e. the function and its first derivative are continuous); see full description .	Results	Files
P ?	vc-objectivity	informational	Total energy is unchanged and forces transform correctly under rigid-body translation and rotation; see full description .	Results	Files
P ?	vc-inversion-symmetry	informational	Total energy is unchanged and forces change sign when inverting a configuration through the origin; see full description .	Results	Files
P ?	vc-memory-leak	informational	The model code does not have memory leaks (i.e. it releases all allocated memory at the end); see full description .	Results	Files
P ?	vc-thread-safe	mandatory	The model returns the same energy and forces when computed in serial and when using parallel threads for a set of configurations. Note that this is not a guarantee of thread safety; see full description .	Results	Files
P ?	vc-unit-conversion	mandatory	The model is able to correctly convert its energy and/or forces to different unit sets; see full description .	Results	Files

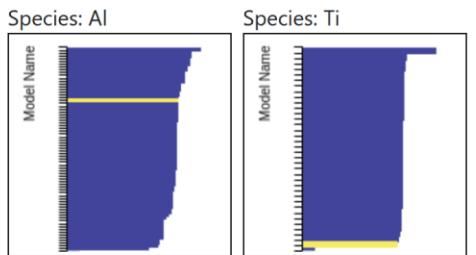
VCs

VISUALIZERS (IN-PAGE)

Visualizers and tables

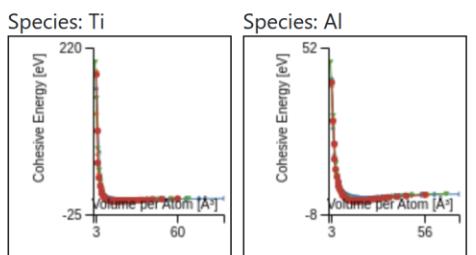
BCC Lattice Constant

This bar chart plot shows the mono-atomic body-centered cubic (bcc) lattice constant predicted by the current model (shown in the unique color) compared with the predictions for all other models in the OpenKIM Repository that support the species. The vertical bars show the average and standard deviation (one sigma) bounds for all model predictions. Graphs are generated for each species supported by the model.



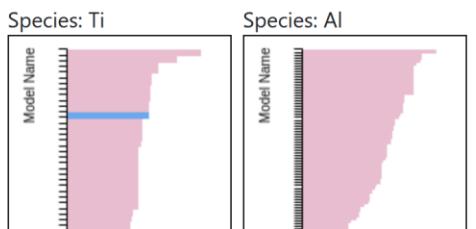
Cohesive Energy Graph

This graph shows the cohesive energy versus volume-per-atom for the current mode for four mono-atomic cubic phases (body-centered cubic (bcc), face-centered cubic (fcc), simple cubic (sc), and diamond). The curve with the lowest minimum is the ground state of the crystal if stable. (The crystal structure is enforced in these calculations, so the phase may not be stable.) Graphs are generated for each species supported by the model.



Diamond Lattice Constant

This bar chart plot shows the mono-atomic face-centered diamond lattice constant predicted by the current model (shown in the unique color) compared with the predictions for all other models in the OpenKIM Repository that support the species. The vertical bars show the average and standard deviation (one sigma) bounds for all model predictions. Graphs are generated for each species supported by the model.



Test results and errors

CohesiveEnergyVsLatticeConstant_TD_554653289799_003

Cohesive energy versus lattice constant curve for monoatomic cubic lattices v003

Creators:

Contributor: karls

Publication Year: 2019

DOI: <https://doi.org/10.25950/64cb38c5>

This Test Driver uses LAMMPS to compute the cohesive energy of a given monoatomic cubic lattice (fcc, bcc, sc, or diamond) at a variety of lattice spacings. The lattice spacings range from a_{\min} ($=a_{\min_frac} \cdot a_0$) to a_{\max} ($=a_{\max_frac} \cdot a_0$) where a_0 , a_{\min_frac} , and a_{\max_frac} are read from stdin (a_0 is typically approximately equal to the equilibrium lattice constant). The precise scaling and number of lattice spacings sampled between a_{\min} and a_0 (a_0 and a_{\max}) is specified by two additional parameters passed from stdin: N_{lower} and $\text{samplesnacing}_{\text{lower}}$ (N_{upper} and $\text{samplesnacing}_{\text{upper}}$). Please see RFADMF.txt for further details.

Test	Test Results	Link to Test Results page	Benchmark time ⓘ
Cohesive energy versus lattice constant curve for bcc Al v004	expand	view	19195
Cohesive energy versus lattice constant curve for bcc Ti v004	expand	view	12870
Cohesive energy versus lattice constant curve for diamond Al v004	expand	view	14233
Cohesive energy versus lattice constant curve for diamond Ti v004	expand	view	15755
Cohesive energy versus lattice constant curve for fcc Al v004	expand	view	13298
Cohesive energy versus lattice constant curve for fcc Ti v004	expand	view	15976
Cohesive energy versus lattice constant curve for sc Al v004	expand	view	21879

ElasticConstantsCubic_TD_011862047401_006

Elastic constants for cubic crystals at zero temperature and pressure v006

Creators: Junhao Li and Ellad Tadmor

Contributor: tadmor

Publication Year: 2019

DOI: <https://doi.org/10.25950/5853fb8f>

Computes the cubic elastic constants for some common crystal types (fcc, bcc, sc, diamond) by calculating the hessian of the energy density with respect to strain. An estimate of the error associated with the numerical differentiation performed is reported.

Test	Test Results	Link to Test Results page	Benchmark time ⓘ
Elastic constants for bcc Al at zero temperature v006	expand	view	2015

FILES

- [CMakeLists.txt](#)
- [LICENSE.CDDL](#)
- [Zope-Ti-Al-2003.eam.alloy](#)
- [kimprovenance.edn](#)
- [kimspec.edn](#)

Download parameter file if you do not wish to use KIM API

DOWNLOAD

EAM_Dynamo_ZopeMishin_2003_TiAl_MO_117656786760_005.txz	Tar+XZ	Linux and OS X archive
EAM_Dynamo_ZopeMishin_2003_TiAl_MO_117656786760_005.zip	Zip	Windows archive

DOWNLOAD DEPENDENCY

This Model requires a Model Driver. Archives for the Model Driver [EAM_Dynamo_MD_120291908751_005](#) appear below.

EAM_Dynamo_MD_120291908751_005.txz	Tar+XZ	Linux and OS X archive
EAM_Dynamo_MD_120291908751_005.zip	Zip	Windows archive

WIKI

Wiki is ready to accept new content.

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Model Drivers
Models
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Page 1 of 1

Test Drivers - Alphabetical

Test Drivers in the OpenKIM Repository

A "test driver" is a computational protocol for computing one or more properties of a system (e.g., energy of a cubic crystal). [Click for more information.](#)

Each test driver is associated with multiple "tests" which fully specify the property and define it for a particular system.

Browse to the new
EquilibriumCrystalStructure
test driver

Test Driver	Title
ClusterEnergyAndForces_TD_000043093022_003	Conjugate gradient relaxation of atomic cluster v003
CohesiveEnergyVsLatticeConstant_TD_554653289799_003	Cohesive energy versus lattice constant curve for monoatomic cubic lattices v003
DislocationCoreEnergyCubic_TD_452950666597_001	Dislocation core energy for cubic crystals at a set of dislocation core cutoff radii v001
ElasticConstantsCubic_TD_011862047401_006	Elastic constants for cubic crystals at zero temperature and pressure v006
ElasticConstantsFirstStrainGradient_TD_361847723785_001	Classical and first strain gradient elastic constants for simple lattices v001
ElasticConstantsHexagonal_TD_612503193866_004	Elastic constants for hexagonal crystals at zero temperature v004
EquilibriumCrystalStructure_TD_457028483760_000	Equilibrium structure and energy for a crystal structure at zero temperature and pressure v000
GrainBoundaryCubicCrystalSymmetricTiltRelaxedEnergyVsAngle_TD_410381120771_003	Relaxed energy as a function of tilt angle for a symmetric tilt grain boundary within a cubic crystal v003
LammpsExample2_TD_887699523131_002	LammpsExample2: energy-volume curve for monoatomic cubic lattice
LammpsExample_TD_567444853524_004	LammpsExample: cohesive energy and equilibrium lattice constant of fcc argon
LatticeConstant2DHexagonalEnergy_TD_034540307932_002	Cohesive energy and equilibrium lattice constant of hexagonal 2D crystalline layers v002
LatticeConstantCubicEnergy_TD_475411767977_007	Equilibrium lattice constant and cohesive energy of a cubic lattice at zero temperature and pressure v007
LatticeConstantHexagonalEnergy_TD_942334626465_005	Equilibrium lattice constants for hexagonal bulk structures at zero temperature and pressure v005
LinearThermalExpansionCoeffCubic_TD_522633393614_001	Linear thermal expansion coefficient of cubic crystal structures v001
PhononDispersionCurve_TD_53019586545_004	Phonon dispersion relations for an fcc lattice v004
StackingFaultFccCrystal_TD_228501831190_002	Stacking and twinning fault energies of an fcc lattice at zero temperature and pressure v002



[2] Esters M, Oses C, Divilov S, Eckert H, Friedrich R, Hicks D, et al. *aflow.org*: A web ecosystem of databases, software and tools. Computational Materials Science [Internet]. 2023;216:111808. Available from: <https://www.sciencedirect.com/science/article/pii/S0927025622005195> doi:10.1016/j.commatsci.2022.111808 ↗

[3] Oses C, Esters M, Hicks D, Divilov S, Eckert H, Friedrich R, et al. *aflow++*: A C++ framework for autonomous materials design. Computational Materials Science [Internet]. 2023;217:111889. Available from: <https://www.sciencedirect.com/science/article/pii/S0927025622006000> doi:10.1016/j.commatsci.2022.111889 ↗

[4] Nikiforov I, Tadmor EB. Equilibrium structure and energy for a crystal structure at zero temperature and pressure v000. OpenKIM; 2023. [doi:10.25950/53ef2ea4](https://doi.org/10.25950/53ef2ea4) ↗

[5] Tadmor EB, Elliott RS, Sethna JP, Miller RE, Becker CA. The potential of atomistic simulation models for predicting equilibrium crystal structures. JOM. 2011;63(7):17. [doi:10.1007/s11837-011-0102-6](https://doi.org/10.1007/s11837-011-0102-6) ↗

[6] Elliott RS, Tadmor EB. Knowledgebase of Interatomic Models (KIM) Application Programming Interface. JOM. 2011;63(7):17. [doi:10.25950/ff8f563a](https://doi.org/10.25950/ff8f563a) ↗

[Click here to download the above citation in BibTeX format.](#)

Funding Not available

Short KIM ID ⓘ TD_457028483760_000

Extended KIM ID ⓘ EquilibriumCrystalStructure_TD_457028483760_000

DOI 10.25950/53ef2ea4
<https://doi.org/10.25950/53ef2ea4>
<https://search.datacite.org/works/10.25950/53ef2ea4>

KIM Item Type Test Driver

Properties ⓘ

- tag:staff@noreply.openkim.org,2023-02-21:property/binding-energy-crystal
- tag:staff@noreply.openkim.org,2023-02-21:property/crystal-structure-npt

KIM API Version 2.2

Simulator Name ⓘ ase

Tests using this Test Driver

[EquilibriumCrystalStructure_A10B3_hP26_194_ahk_h_ALMn_TE_188364898751_000](#)

Click to see the *property definition(s)* the tests using this driver report

Click on any test using this driver



compounds the 'binding-potential-energy-per-formula' will depend on the stoichiometric formula, e.g. for MoS₂ (AB₂-type compound) the energy is per MoS₂ unit (i.e. 3 times larger than the 'binding-potential-energy-per-atom` value). The reported energies are actual energies (not the negative of the energy as commonly reported), therefore these values will be negative for a crystal that is more stable than its isolated constituents.

Contributor ?	ilia
Maintainer ?	ilia
Creation date ?	2023-02-21
Content on GitHub ?	Property Definition Physics Validator Property Documentation Wiki

See the [KIM Properties Framework](#) for more detailed information.

Jump below to [Property Documentation Wiki](#) content

Property Definition Keys

Jump to:

Required

- a
- binding-potential-energy-per-atom
- binding-potential-energy-per-formula
- prototype-label
- stoichiometric-species

Optional

- library-prototype-label
- parameter-names
- parameter-values
- short-name

**Keys in this property
(useful for querying)**



MODELS

EAM_Dynamo_MD_120291908751_005

Model	Test Results	Link to Test Results page	Benchmark time ⓘ
EAM_Dynamo_SchopfBrommerFrigan_2012_AlMnPd_MO_137572817842_000	✖ collapse	🔍 view	71854
instance-id: 1			
Equilibrium crystal structure and binding potential energy at zero temperature and applied stress (For more information, see the property definition binding-energy-crystal)			
AFLOW prototype label = A10B3_hP26_194_ahk_h Species = ["Al" "Mn"] a = 7.5156 angstrom Other parameter names = ["c/a" "x2" "x3" "x4" "z4"] Other parameter values = [1.0103252 0.5452406 0.88240115 0.79605205 0.9315291] AFLOW library prototype = --'			

Click to see a detailed result page with all output files

Click to see a summary of a test result

EAM_IMD_MD_113599595631_003

Model	Test Results	Link to Test Results page	Benchmark time ⓘ
EAM_IMD_SchopfBrommerFrigan_2012_AlMnPd_MO_878712978062_003	✖ expand	🔍 view	154750

LJ_MD_414112407348_003

Model	Test Results	Link to Test Results page	Benchmark time ⓘ
LJ_ElliottAkerson_2015_Universal_MO_959249795837_003	⚠️	✖ expand	601315

ERRORS



OpenKIM Query

Simplified interface
for Test Results only

Get Test Result

Raw Query

Reset

Examples

Basic usage

Specifying SI units

Retrieving multiple keys

Test:

```
["LatticeConstantCubicEnergy_diamond_Si_TE_849680434885"]
```

A square-bracketed list containing the Test name. The following formats are accepted: ["CC_DDDDDDDDDDDDD"], ["TestName_CC_DDDDDDDDDDDDD"], ["CC_DDDDDDDDDDD_VVV"], ["TestName_CC_DDDDDDDDDDD_VVV"]. Generally, the three digit version extension (VVV) should be omitted so that the latest version of the Test will be queried on. For more on KIM IDs, refer to the [Guide to KIM IDs](#).

Model:

```
["EDIP_JustoBazantKaxiras_1998_Si_MO_958932894036"]
```

Accepted formats are identical to those above and, similar to above, the three digit version extension should generally be omitted.

Species:

```
["Si"]
```

A square-bracketed, comma-separated list of quoted strings corresponding to standard elemental symbols (case sensitive). Test Results returned will be required to contain each element listed.

Property:

```
["cohesive-potential-energy-cubic-crystal"]
```

A square-bracketed list containing the property name. May be specified as either the short name of a Property Definition, e.g. structure-cubic-crystal-npt, or the full property ID, e.g. ["tag:staff@noreply.openkim.org,2014-04-15:property/structure-cubic-crystal-npt"]. Only the short name should generally be used so that the latest version of the Property Definition is queried on. See [here](#) for a current list of Property Definitions.

Keys:

```
["a", "cohesive-potential-energy"]
```

Ordered array of keys specified as a square-bracketed, comma-separated list of quoted strings. The order of the keys must correspond to the order of the entries in the 'Units' field below.

Units:

```
["angstrom", "eV"]
```

A square-bracketed, comma-separated list of quoted strings indicating the desired units that the value of each key should be returned in. The order of the entries in this list should correspond to the order of the entries in the 'Keys' field above. Valid strings for units are any of those recognized by the [GNU units](#) utility, or the special string "SI". Keys which are unitless must have a value of null (case-sensitive and unquoted).

Scroll down to see results and syntax for programmatic use (in “raw query” mode as well)

["angstrom"]
Ordered array of keys specified as a square-bracketed, comma-separated list of quoted strings. The order of the keys must correspond to the order of the entries in the 'Units' field below.

Units:

["angstrom"]

A square-bracketed, comma-separated list of quoted strings indicating the desired units that the value of each key should be returned in. The order of the entries in this list should correspond to the order of the entries in the 'Keys' field above. Valid strings for units are any of those recognized by the [GNU units](#) utility, or the special string "SI". Keys which are unitless must have a value of null (case-sensitive and unquoted).

Submit

Results

[5.430497780442238]

Query Link

https://query.openkim.org/get_test_result?test=%5B%22LatticeConstantCubicEnergy_diamond_Si__TE_849680434885%22%5D&model=%5B%22EDIP_JustoBazantKaxiras_1%22%5D

Curl

```
curl --data-urlencode 'test=[ "LatticeConstantCubicEnergy_diamond_Si__TE_849680434885" ]' --data-urlencode 'model=[ "EDIP_JustoBazantKaxiras_1" ]'
```

GET

https://query.openkim.org/api/get_test_result?test=%5B%22LatticeConstantCubicEnergy_diamond_Si__TE_849680434885%22%5D&model=%5B%22EDIP_JustoBazantKaxiras_1%22%5D

Python

```
result = requests.post("https://query.openkim.org/api/get_test_result",data={'test': '[ "LatticeConstantCubicEnergy_diamond_Si__TE_849680434885" ]', 'model': '[ "EDIP_JustoBazantKaxiras_1" ]'})
```

d3

```
d3.json('https://query.openkim.org/api/get_test_result?test=%5B%22LatticeConstantCubicEnergy_diamond_Si__TE_849680434885%22%5D&model=%5B%22EDIP_JustoBazantKaxiras_1%22%5D')
```

jQuery

```
$.post("https://query.openkim.org/api/get_test_result",{"test": "[ \"LatticeConstantCubicEnergy_diamond_Si__TE_849680434885\" ]", "model": "[ \"EDIP_JustoBazantKaxiras_1998_Si__MO_95893289403\" ]"});
```

pipeline.stdin.tpl

```
@< get_test_result(test=[ "LatticeConstantCubicEnergy_diamond_Si__TE_849680434885" ], model=[ "EDIP_JustoBazantKaxiras_1998_Si__MO_95893289403" ]) >
```

[Get Test Result](#)[Raw Query](#)[Reset](#)

Raw Mongo query – powerful but complex

Pre-filled examples

Examples

[Get all jobs that are currently running](#)[Get all Test Drivers in the database](#)[Get all fcc Al lattice constants and the Model that ran them](#)[Longest running Test name and time](#)[Get a 10 line tail of the logs](#)[Get the lowest energy crystal structure for each Model using Al](#)

query

```
1 { "meta.type": "tr", "property-id": "tag:staff@noreply.openkim.org,2014-04-15:property/structure-cubic-crystal-npt", "meta.runner.kimcode": "
```

Things you want true, as a dictionary of key value pairs, e.g. {"type": "td"} makes sure that all objects are test drivers.

fields

```
1 { "a.source-value": 1, "meta.subject.kimcode": 1}
```

Things you want back, as a dictionary of booleans, e.g. {"type":1, "path":1} returns just type and path (and '_id')

aggregate

```
1
```

“obj” for KIM items,
“data” for test results
and reference data

A mongodb aggregation pipeline. Use \$sort, \$limit, \$skip, and \$distinct aggregation pipeline stages instead of entering in their respective fields below if using aggregate(). For more information, check the [docs](#)

database

```
data
```

Database you want, valid options are [obj, data, job, log, agent]

distinct

```
[distinct]
```

Things you want distinct, just a key, e.g. "type" would return distinct type fields. Note, this doesn't play well with others.

A mongodb aggregation pipeline. Use \$sort, \$limit, \$skip, and \$distinct aggregation pipeline stages instead of entering in their respective fields below if using aggregate(). For more information, check the [docs](#)

database

[data]

Database you want, valid options are [obj, data, job, log, agent]

sort

[[{"inserted_on": -1}]]

Things you want sorted on, as a string, or a list with direction, e.g. "Kimcode" sorts on Kimcode, [{"kimcode": -1}] gives reverse kimcode

limit

3

How many you want, an integer, how it stops, leave empty for all

skip

[skip]

How many you want to skip, relevant if ordered

distinct

[distinct]

Things you want distinct, just a key, e.g. "type" would return distinct type fields. Note, this doesn't play well with others.

project

[project]

Reduce result to an array where the columns are ordered by this list i.e. [{"meta.kimcode": "crystal-structure.a.source"}]

flatten



Whether or not to

This will give you most recent data

history



Return full database history. By default, only returns latest data

count



Return only count of number results created by query

Submit

Results

```
[  
  {  
    "a.source-value": 4.032082748413087,  
    "meta.subject.kimcode": "EAM_CubicNaturalSpline_ErcolelliAdams_1994_A1_MO_800509458712_002"  
  },  
  {  
    "a.source-value": 4.05000071525574,  
    "meta.subject.kimcode": "EAM_Dynamo_AngeloMoodyBaskes_1995_NiAlH_MO_418978237058_005"  
  },  
  {  
    "a.source-value": 4.05000071525574,  
    "meta.subject.kimcode": "EAM_Dynamo_AngeloMoodyBaskes_1995_NiAlH_MO_418978237058_005"  
  }]
```

Set a low limit while playing around



My strategy:

- Find an example that's related to what you want
- Make it as loose as possible
- Set a low limit
- Look through the results to see how the data is structured
- Decide what to query for and which fields to request
- Read the Mongo documentation
- Use Google

query

```
1 {"meta.type": "tr"}
```

Things you want true, as a dictionary of key value pairs, e.g. {"type": "td"} makes sure that all objects are test drivers.

fields

```
1
```

Things you want back, as a dictionary of booleans, e.g. {"type":1, "path":1} returns just type and path (and '_id')

aggregate

```
1
```

A mongodb aggregation pipeline. Use \$sort, \$limit, \$skip, and \$distinct aggregation pipeline stages instead of entering in their respective fields below if using aggregate(). For more information, check the [docs](#)

database

data

Database you want, valid options are [obj, data, job, log, agent]

sort

```
["inserted_on",-1]
```

Things you want sorted on, as a string, or a list with direction, e.g. "kimcode" sorts on kimcode, `["kimcode", -1]` gives reverse kimcode

limit

```
3
```

How many you want, an integer, how it stops, leave empty for all

skip

distinct

[distinct]

Things you want distinct, just a key, e.g. "type" would return distinct type fields. Note, this doesn't play well with others.

project

[project]

Reduce result to an array where the columns are ordered by this list i.e. ["meta.kimcode", "crystal-structure.a.source-value"]. Implies flatten.

flatten



Whether or not to flatten the keys in the dictionary

history

KIM Model Comparison Tool

Select KIM Models to Compare

al

Compare

- EAM_ErcolessiAdams_1994 AI _MO_324507536345_003
- EAM_Dynamo_Zhakhovsky_2009 AI _MO_519613893196_000
- EAM_Dynamo_ZopeMishin_2003 AI _MO_664470114311_005
- EAM_Dynamo_SturgeonLaird_2000 AI _MO_120808805541_005
- EAM_Dynamo_ErcolessiAdams_1994 AI _MO_123629422045_005
- MEAM_LAMMPS_LeeShimBaskes_2003 AI _MO_353977746962_000
- EAM_Dynamo_MishinFarkasMehl_1999 AI _MO_651801486679_005

compare.openkim.org
(beta version, no
navigation from main
site yet)

Getting Started

- [Guide to Getting Started with KIM](#)

About

- [About KIM](#)
- [Documentation](#)
- [2018 Survey Results](#)
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- [KIM API](#)
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- [Contribute Other Content](#)

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- [EDN Format](#)

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- [Model Drivers](#)
- [Models](#)
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- [Tests](#)
- [Verification Checks](#)
- [Reference Data](#)
- [Query the KIM Repository](#)
- [KIM Property Definitions](#)
- [Property Table](#)

KIM Model Comparison

Models:

- [EAM_Dynamo_ErcolessiAdams_1994_Al_N](#)
- [MEAM_LAMMPS_LeeShimBaskes_2003_Al_N](#)
- [Morse_Shifted_GirifalcoWeizer_1959MedC](#)

[View more example model combinations](#)

Material Properties

[Comparison & Errors](#)[+ Add Property](#)

Add Property

A Property Definition is
[crystal](#) Property Definition
basis atom coordinate

View a list of all properties

Property ID

binding-energy-crystal
bulk-modulus-isothermal-cubic-crystal-npt
cohesive-energy-relation-cubic-crystal
cohesive-potential-energy-cubic-crystal
cohesive-potential-energy-hexagonal-crystal
crystal-structure-npt
elastic-constants-isothermal-cubic-crystal-npt
extrinsic-stacking-fault-relaxed-energy-fcc-crystal-npt
gamma-surface-relaxed-fcc-crystal-npt
grain-boundary-symmetric-tilt-energy-relaxed-relation-cubic-crystal
intrinsic-stacking-fault-relaxed-energy-fcc-crystal-npt
linear-thermal-expansion-coefficient-cubic-crystal-npt
phonon-dispersion-dos-cubic-crystal-npt
phonon-dispersion-relation-cubic-crystal-npt
stacking-fault-relaxed-energy-curve-fcc-crystal-npt
structure-cubic-crystal-npt
structure-hexagonal-crystal-npt
surface-energy-broken-bond-fit-cubic-bravais-crystal-npt

Select a Property ID from above to get started.

Choose a property to compare
among chosen models



KIM Model Comparison

Models:

- [EAM_Dynamo_ErcolessiAdams_1994_Al_N](#)
- [MEAM_LAMMPS_LeeShimBaskes_2003_Al_N](#)
- [Morse_Shifted_GirifalcoWeizer_1959MedC](#)

[View more example model combinations](#)

Material Properties

[Comparison & Errors](#)[+ Add Property](#)

Add Property

A Property Definition is
[crystal](#) Property Definition
basis atom coordinate

View a list of all properties

Property ID

binding-energy-crystal
bulk-modulus-isothermal-cubic-crystal-npt
cohesive-energy-relation-cubic-crystal
cohesive-potential-energy-cubic-crystal
cohesive-potential-energy-hexagonal-crystal
crystal-structure-npt
elastic-constants-isothermal-cubic-crystal-npt
extrinsic-stacking-fault-relaxed-energy-fcc-crystal-npt
gamma-surface-relaxed-fcc-crystal-npt
grain-boundary-symmetric-tilt-energy-relaxed-relation-cubic-crystal
intrinsic-stacking-fault-relaxed-energy-fcc-crystal-npt
linear-thermal-expansion-coefficient-cubic-crystal-npt
phonon-dispersion-dos-cubic-crystal-npt
phonon-dispersion-relation-cubic-crystal-npt
stacking-fault-relaxed-energy-curve-fcc-crystal-npt
structure-cubic-crystal-npt
structure-hexagonal-crystal-npt
surface-energy-broken-bond-fit-cubic-bravais-crystal-npt

Select a Property ID from above to get started.

Choose a property to compare
among chosen models



Name the tab

Custom Query Label

FCC Binding Energy

This appears in the tabs on the left to help you navigate your results. The default label for the Property Query is the Property short name. Customize this for your data.

Match Keys

These keys are used to filter the set of all material properties computed by the selected models, retaining only those properties that share the same value for them.

prototype-label: Prototype label (not including an enumeration suffix) as defined by the AFLOW standard (e.g. 'A_tI4_141_a') for the structure. It is expected that the alphabetically lowest of all equivalent labels is chosen.

short-name: Commonly used name associated with the 'library-prototype-label' key according to the AFLOW prototype library (e.g. 'Face-Centered Cubic' or 'Molybdenite').

stoichiometric-species: Element symbols corresponding to the atom types in the stoichiometric formula which appears at the start of the prototype label (e.g. ['Mo','S'] for the AB₂ stoichiometric formula, means that the 'A' atom is 'Mo' and the 'B' atom is 'S' for the MoS₂ structure).

Choose a combination of Match Keys and values from the options below:

prototype-label: A_cF4_225_a
short-name: Face-Centered Cubic
stoichiometric-species: ['Al']

Click to select

prototype-label: A_ci2_229_a
short-name: Body-Centered Cubic
stoichiometric-species: ['Al']

Click to select

Test Driver

EquilibriumCrystalStructure_TD_457028483760_000

A Test Driver is a code that can be used to perform a material property calculation under different conditions, e.g. a range of species, structures, temperatures, etc., with each such combination corresponding to a different Test that uses the driver. For example, the same Test Driver may be used by one Test that computes the lattice constant of diamond silicon and another that computes the lattice constant of fcc copper.

Add the comparison

Add Material Property Comparison



Add another tab

Material Properties

FCC Binding Energy

Remove this Property

FCC Binding Energy

Comparison & Errors

+ Add Property

Material Property Details

Property	tag:staff@noreply.openkim.org,2023-02-21:property/binding-energy-crystal
Title	Equilibrium crystal structure and binding energy at zero temperature and applied stress
Test Driver	EquilibriumCrystalStructure_TD_457028483760_000
Match key	prototype-label=A_cF4_225_a
Match key	short-name=Face-Centered Cubic
Match key	stoichiometric-species=['Al']

Comparison of property fields

Model Comparison Table

Model	a lattice constant (angstrom)	Crystal prototype parameter values (undefined)	Binding potential energy per formula (eV)	Binding potential energy per atom (eV)	Test Result	
					link	link
A EAM_Dynamo_ErcolessiAdams_1994_Al_MO_123629422045_005	4.032100		-3.360000	-3.360000	link	
B MEAM_LAMMPS_LeeShimBaskes_2003_Al_MO_353977746962_000	4.044700		-3.360000	-3.360000	link	
C Morse_Shifted_GirfalcoWeizer_1959MedCutoff_Al_MO_279544746097_004	4.039800		-2.888341	-2.888341	link	

Matching reference data

Reference Data Table

Property	Reference Data			Raw Data	Description
	Ave	STD	Unit	Choose to select all of ...	
a lattice constant	4.04	0.00	angstrom	4.039 <input checked="" type="checkbox"/> RD_111652753638_000 (C) 4.039 <input checked="" type="checkbox"/> RD_118257218774_000 (C) 4.039 <input checked="" type="checkbox"/> RD_200592182295_000 (C) 4.039 <input checked="" type="checkbox"/> RD_241135774038_000 (C) 4.039 <input checked="" type="checkbox"/> RD_370685119673_000 (C) 4.039 <input checked="" type="checkbox"/> RD_476650713938_000 (C)	The equilibrium 'a' lattice constant of the crystal structure as defined by the AFLOW standard. Relative values of other lattice parameters (if present) are given in the 'parameter-values' key.



KIM Model Comparison Tool

Models:

- [EAM_Dynamo_ErcolessiAdams_1994_Al_MO_123629422045_005](#)
- [MEAM_LAMMPS_LeeShimBaskes_2003_Al_MO_353977746962_000](#)
- [Morse_Shifted_GirifalcoWeizer_1959MedCutoff_Al_MO_279544746097_004](#)

[View more example model combinations](#)

[Start New Comparison](#)

Click
here
and
choose
[sz93tn](#)

Material Properties

FCC Binding Energy

[Remove this Property](#)

FCC Binding
Energy

Comparison &
Errors

[+ Add Property](#)

Material Property Details

Property [tag:staff@noreply.openkim.org,2023-02-21:property/binding-energy-crystal](#)

Title Equilibrium crystal structure and binding energy at zero temperature and applied stress

Test Driver [EquilibriumCrystalStructure_TD_457028483760_000](#)

Match key prototype-label=A_cF4_225_a

Match key short-name=Face-Centered Cubic

Match key stoichiometric-species=['Al']

Model Comparison Table

Parameter name (angstrom)	Parameter values (undefined)	Total energy per formula (eV)	Total energy per atom (eV)



FCC Binding
Energy

FCC Bulk Modulus

FCC Elastic
Constants

Comparison &
Errors

+ Add Property

Combined
comparison
w/reference
data and
timing

Combined Material Property Comparisons

Model	Reference Data Ave ± STD	FCC Binding Energy			FCC Bulk Modulus			FCC Elastic Constants		
		a lattice constant	Binding potential energy per atom	Binding potential energy per formula unit	Total crystal prototype parameter value	Lattice constant a	Isothermal bulk modulus	Lattice constant a	Isothermal bulk modulus	Test Result
A	EAM_Dynamo_ErcoliessAdams_1994_AI_MO_123629422045_005	4.032100 (0.17%)	-3.360000 (10.25%)	-3.360000 (10.25%)	4.032082 (0.17%)	80.797803 (2.98%)	11 (8)			
B	MEAM_LAMMPS_LeeShimBaskes_2003_AI_MO_353977746962_000	4.044700 (0.14%)	-3.360000 (10.25%)	-3.360000 (10.25%)	4.044651 (0.14%)	79.388444 (4.67%)	11 (5)			
C	Morse_Shifted_GirifalcoWeizer_1959MedCutoff_AI_MO_279544746097_004	4.039800 (0.02%)	-2.888341 (22.85%)	-2.888341 (22.85%)	4.039798 (0.02%)	76.620705 (7.99%)	95 (1)			

The reference data values are set in the Material Properties tabs. There all available reference data is displayed, and the user can choose which reference data values to use when computing errors.

The background color of a model prediction is shown as green, yellow, and red indicating increasing relative error according to a scale set by the user. The default is green under a 10% error, yellow under 40%, and red above that.

Click to view calculations



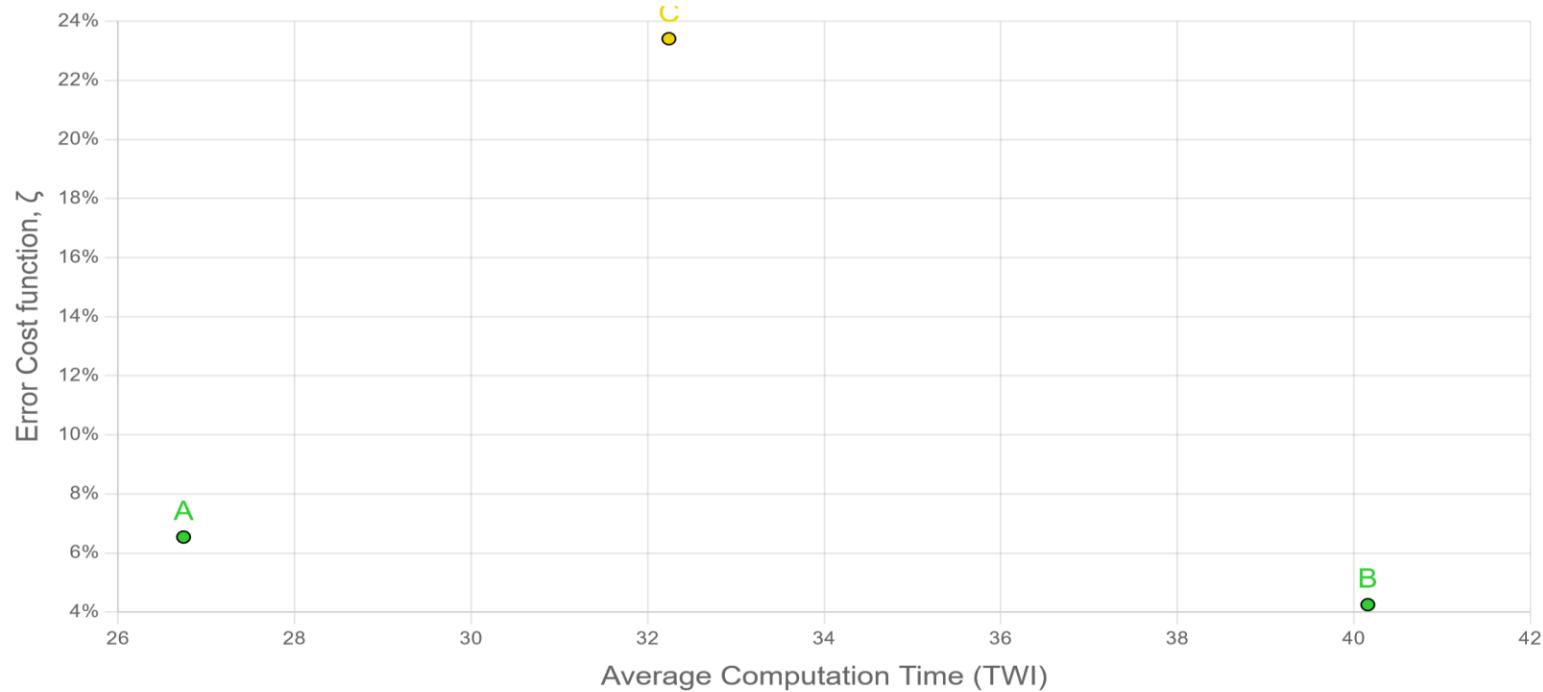
You may change the background color threshold of a model prediction here:

10

Low Error Threshold (Percent)



Error Cost vs Computation Time



You may hover over a point in the plot above to view the exact value.

[Click to view detailed explanation](#)

Assign
error
weights

Weight Assignment Table

FCC Binding Energy	lattice constant	binding potential energy per atom	binding potential energy per formula	FCC Bulk Modulus	FCC Elastic Constants
				lattice constant a	lthermal bulk modulus lthermal C11 lthermal C12 lthermal C44



Hands-on tutorial

- Binder repo:
 - <https://github.com/openkim/openkim-demo>
 - Click the “launch binder” icon: A rectangular button with a dark grey background and a light blue right side. It features a small circular icon with a white 'b' inside on the left, followed by the words 'launch' and 'binder' in white.
 - The repo also contains a PDF of these slides



Questions and Exercises

- Feel free to experiment and ask questions
- Suggested exercises:
 - Download a different potential and modify the LAMMPS input files and/or ASE scripts to run with it, possibly using a different lattice type.
 - Try plotting the convex hull with different potentials. Are any of them particularly bad? Navigate to their OpenKIM page and see if you can figure out why.
 - Find the most recent errors that were reported by the pipeline. Navigate to them through the test or model pages and examine why they occurred. (Hints: {"meta.type":"er"}
[["inserted_on",-1]])

