

OpenKIM for the LAMMPS User

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PIs and Key Collaborators:

- Ellad Tadmor (UMN), KIM Director
- Ryan Elliott (UMN), KIM Technical Lead
- Mark Transtrum (BYU), Co/PI
- George Karypis (UMN), Co/PI
- Ronald Miller (Carleton), KIM Editor
- Hendrik Heinz (Boulder), PI (Cyberloop)
- Wonpil Im (Lehigh), Co/PI (Cyberloop)
- Stefano Martiniani (UMN), Co/PI (Colabfit)

Core Developers

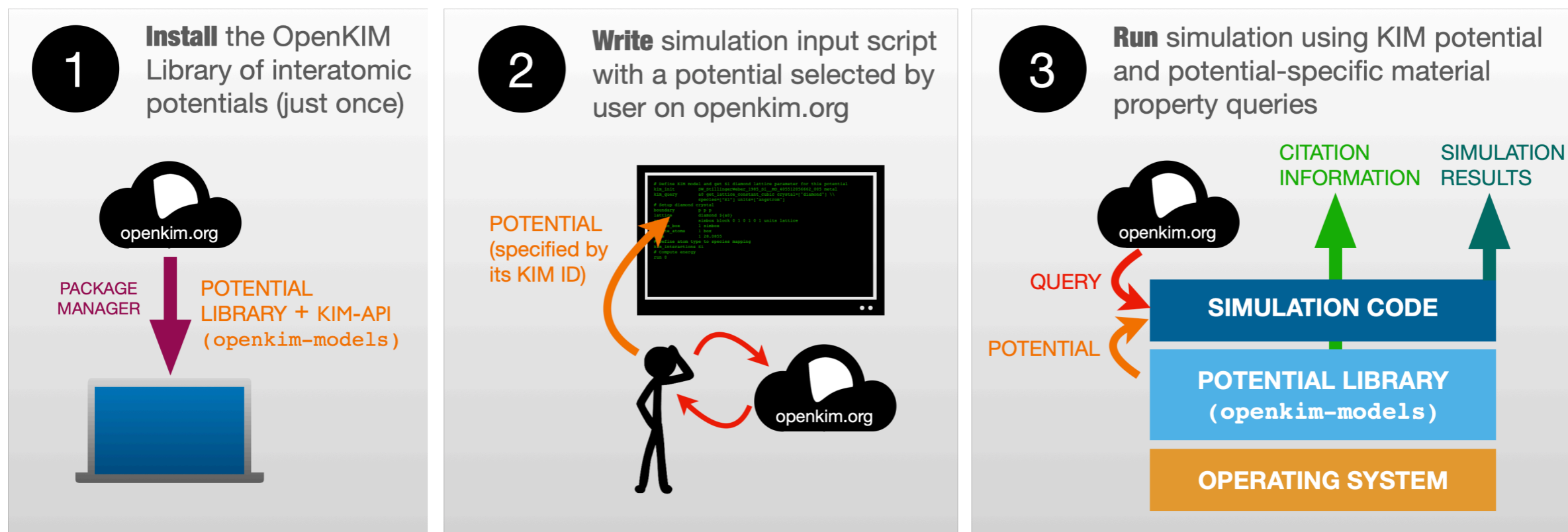
- Yaser Afshar (UMN)
- Daniel S. Karls (UMN)
- Petros Karypis (UMN)
- Yonatan Kurniawan (BYU)
- Saurav Manchanda (UMN)
- Cody Petrie (BYU)
- Zeren Shui (UMN)
- Mingian Wen (LBL)



Funding through the US National Science Foundation

NSF CMMT (2019-)

Open Knowledgebase of Interatomic Models (OpenKIM)



OpenKIM by the Numbers (10-Aug-2021)

- 543 interatomic potentials
- 2613 property tests
- 10 verification checks
- 74,899 reference data items
- 15 KIM-compliant platforms
- 710 registered users in 50 countries

Models Tests [Contribute a Model](#)

Models

Click on an element to find interatomic models for that species. You can narrow the selection to models that support multiple species after you click.

H	Sp																			He
Li	Be										B	C	N	O	F	Ne				
Na	Mg										Al	Si	P	S	Cl	Ar				
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe			
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn			
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	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						

<https://openkim.org>

Installing the KIM API and library of KIM potentials

Installation from binary

```
# MacOS  
$ brew install lammps openkim-models
```

← This automatically installs KIM API as a dependency

```
# Ubuntu  
$ sudo apt-get install lammps libkim-api-dev openkim-models
```

```
# Conda  
$ conda install lammps kimp openkim-models
```

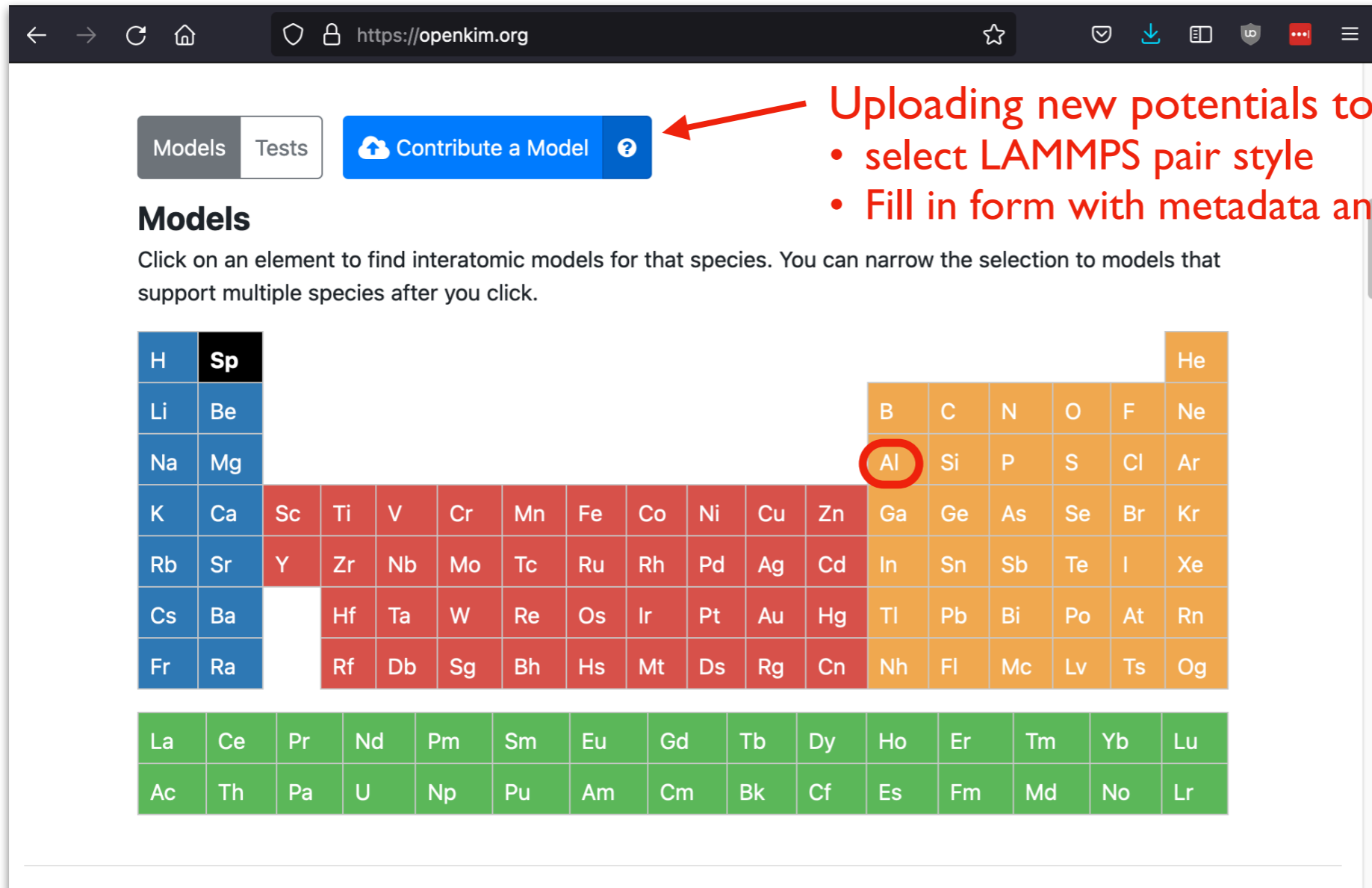
Similar procedures for openSUSE, Fedora, FreeBSD, AUR, CentOS, Debian, ... soon for Windows.
See <https://openkim.org/doc/usage/obtaining-models>

Installation from source

```
# Download latest kim-api package from https://openkim.org/kim-api  
$ cd kim-api-2.2.1  
$ mkdir build  
$ cd build  
$ cmake .. -DCMAKE_BUILD_TYPE=Release  
$ make  
$ sudo make install  
$ sudo ldconfig  
$ kim-api-collections-management install system OpenKIM
```

```
# Download latest lammps package from https://www.lammps.org/download.html  
$ cd lammps  
$ mkdir build  
$ cd build  
$ cmake ../cmake -DPKG_KIM=ON  
$ make
```

Select an OpenKIM Potential



The screenshot shows the OpenKIM website interface. At the top, there are navigation tabs for 'Models' and 'Tests', and a prominent blue button labeled 'Contribute a Model' with a question mark icon. A red arrow points from the text 'Uploading new potentials to OpenKIM is easy:' to this button. Below the navigation, the 'Models' section is active, with a sub-header 'Models' and a brief instruction: 'Click on an element to find interatomic models for that species. You can narrow the selection to models that support multiple species after you click.' Below this is a periodic table where the element 'Al' (Aluminum) is circled in red. The periodic table is color-coded: blue for s-block, red for d-block, orange for p-block, and green for f-block.

Uploading new potentials to OpenKIM is easy:

- select LAMMPS pair style
- Fill in form with metadata and provide param files

Select an OpenKIM Potential

The screenshot shows the OpenKIM website interface. At the top, there is a navigation bar with 'Models' and 'Tests' tabs, and a prominent blue 'Contribute a Model' button with a question mark icon. Below this, the 'Models' section is active, displaying a periodic table where certain elements are highlighted in red (Sc, Ti, V, Y, Zr, Nb, Hf, Ta, Rf, Db) and others in green (La, Ce, Pr, Nd, Ac, Th, Pa, U). A red arrow points from the 'Contribute a Model' button to the text on the right.

Uploading new potentials to OpenKIM is easy:

- select LAMMPS pair style
- Fill in form with metadata and provide param files

The screenshot shows the 'Models - by Species' page on OpenKIM. The page has a navigation menu at the top and a sidebar with links like 'Model Drivers', 'Models', 'Test Drivers', etc. The main content area shows a search filter 'Narrow species selection:' with a dropdown menu set to 'Al'. Below the filter, a table lists various interatomic models. A red arrow points to the 'Al' filter, and another red arrow points to a specific model entry in the table.

Extended KIM ID	Simulator	Title
EAM_CubicNaturalSpline_ErcolessiAdams_1994_AI_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_AiCu_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_AI_MO_123629422045_005	Any	EAM potential (LAMMPS cubic hermite tabulation) for Al developed by Ercolessi and Adams (1994) v005
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

Narrow selection for multiple species (if desired)

Select an OpenKIM Potential

EAM_Dynamo_ErcolessiAdams_1994_AI_MO_123629422045_005
 Interatomic potential for Aluminum (Al)

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

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.

Disclaimer
 By design, this potential is not expected to be accurate for geometries with extremely low coordination -- such as small molecules -- which were not included in the input set.

Contributor
 Ryan S. Elliott

Maintainer
 Ryan S. Elliott

Publication Year
 2016

How to Cite
 This Model originally published in [1] is archived in OpenKIM [2-5].

Verification Check Dashboard

Grade	Name	Category	Brief Description	Full Results	Alert
A	vc-forces-numerical-derivative	mandatory	The model supports all species it claims to support; see full description.	Results	Files
N/A	vc-periodicity-support	mandatory	Periodic boundary conditions are handled correctly; see full description.	Results	Files
A	vc-permutation-symmetry	mandatory	Total energy and forces are unchanged when swapping atoms of the same species; see full description.	Results	Files
A	vc-forces-numerical-derivative	consistency	Forces computed by the model agree with numerical derivatives of the energy; see full description.	Results	Files
F	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
A	vc-objectivity	informational	Total energy is unchanged and forces transform correctly under rigid body translation and rotation; see full description.	Results	Files
A	vc-inversion-symmetry	informational	Total energy is unchanged and forces change sign when inverting a configuration through the origin; see full description.	Results	Files
A	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
A	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
A	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

Visualizers (in-page)

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 signal bar) 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 model 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.

Cubic Crystal Basic Properties Table

Model	ModelID	Lattice Constant [Å]	Cohesive Energy [eV/atom]	c11 [GPa]	c12 [GPa]	c44 [GPa]
EAM	EAM_Dynamo_ErcolessiAdams_1994_AI_MO_123629422045_005	3.1474773108959204	3.307015988617005	88.30540913292008	88.71596661921012	62.94038764918322
EAM	EAM_Dynamo_ErcolessiAdams_1994_AI_MO_123629422045_005	3.998299837112427	2.4887521418963768	N/A	N/A	N/A
EAM	EAM_Dynamo_ErcolessiAdams_1994_AI_MO_123629422045_005	4.03268333157349	3.36000118355623	117.9688302350432	62.21234572721029	36.834998748647
EAM	EAM_Dynamo_ErcolessiAdams_1994_AI_MO_123629422045_005	2.754772530080604	3.005788888207347	132.4956481071132	86.74601088832884	-9.551348075122919

Tests

Disclaimer From Model Developer
 By design, this potential is not expected to be accurate for geometries with extremely low coordination -- such as small molecules -- which were not included in the input set.

CohesiveEnergyVersusVolumePerAtomConstantCurveForMonatomicCubicLatticesV005
 Cohesive energy versus volume-per-atom for monatomic cubic lattices v005

Tests

Test	Test Results	Link to Test Results page	Benchmark time
Cohesive energy versus volume-per-atom for bcc Al v005	Passed	View	1907
Cohesive energy versus volume-per-atom for fcc Al v005	Passed	View	1887
Cohesive energy versus volume-per-atom for sc Al v005	Passed	View	2164
Cohesive energy versus volume-per-atom for diamond Al v005	Passed	View	2847

Wiki
 Wiki is ready to accept new content.

← **KIM ID** **EAM_Dynamo_ErcolessiAdams_1994_AI_MO_123629422045_005**

Metadata:

- Title, description, contributor, species
- Disclaimer
- Citation, DOI, funding, ...

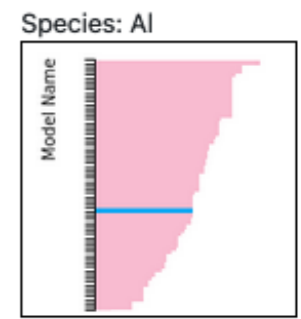
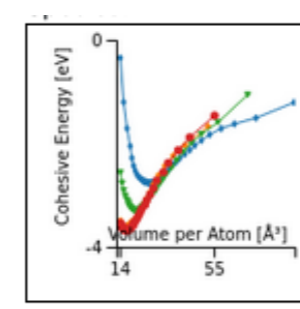
Verification Check (VC) dashboard

- Pass/fail or A-F grades on various VCs
- force numerical derivative, continuity, memory leaks, ...

A	vc-forces-numerical-derivative	consistency	Forces computed by the model agree with numerical derivatives of ..	Results	Files
F	vc-dimer-continuity-c1	informational	The energy versus separation relation of a pair of atoms is C1 ..	Results	Files

Visualizers

- Visual representation of different property calculations
- cohesive energy, crystal structure, elastic constants, ...
- Tabular data



Tests

- Predictions of the potential for many material properties
- cohesive energy, crystal structure, elastic constants, GB energy, dislocation core energy, phonons, ...

← **Wiki** where users can add their comments about the potential.

KIM Basic Usage

Example: Calculate cohesive energy of fcc Al using Ercolessi-Adams EAM

```
units metal
boundary p p p
variable a0 equals 4.05
lattice fcc ${a0}
region simbox block 0 1 0 1 0 1 units lattice
create_box 1 simbox
create_atoms 1 box
mass 1 1.0
pair_style eam/alloy
pair_coeff * * Al_EA.eam.alloy
run 0
```

```
kim init EAM_Dynamo_ErcolessiAdams_1994_Al_MO_123629422045_005 metal
boundary p p p
variable a0 equals 4.05
lattice fcc ${a0}
region simbox block 0 1 0 1 0 1 units lattice
create_box 1 simbox
create_atoms 1 box
mass 1 1.0
kim interactions Al
run 0
```

Only modifications needed to run with OpenKIM potential

KIM Citation Information

Citation information is provided when using KIM potentials.

```
...
Created 4 atoms
  create_atoms CPU = 0.000 seconds

CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE

Your simulation uses code contributions which should be cited:
- OpenKIM: https://doi.org/10.1007/s11837-011-0102-6
- OpenKIM potential: https://openkim.org/cite/MO\_123629422045\_005#item-citation
The log file lists these citations in BibTeX format.

CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE

Neighbor list info ...
...
```

The **log.lammps** file contains all citations in BibTeX format.

How to Cite This Model originally published in [1] is archived in OpenKIM [2-5].

[1] Ercolessi F, Adams JB. Interatomic Potentials from First-Principles Calculations: The Force-Matching Method. *Europhysics Letters*. 1994;26(8):583. [doi:10.1209/0295-5075/26/8/005](https://doi.org/10.1209/0295-5075/26/8/005) — (Primary Source) ⓘ

[2] EAM potential (LAMMPS cubic hermite tabulation) for Al developed by Ercolessi and Adams (1994) v005. OpenKIM; 2018. [doi:10.25950/7cd2a6ab](https://doi.org/10.25950/7cd2a6ab)

[3] EAM Model Driver for tabulated potentials with cubic Hermite spline interpolation as used in LAMMPS v005. OpenKIM; 2018. [doi:10.25950/68defa36](https://doi.org/10.25950/68defa36)

[4] Tadmor EB, Elliott RS, Sethna JP, Miller RE, Becker CA. The potential of atomistic simulations and the Knowledgebase of Interatomic Models. *JOM*. 2011;63(7):17. [doi:10.1007/s11837-011-0102-6](https://doi.org/10.1007/s11837-011-0102-6)


[5] Elliott RS, Tadmor EB. Knowledgebase of Interatomic Models (KIM) Application Programming Interface (API). OpenKIM; 2011. [doi:10.25950/ff8f563a](https://doi.org/10.25950/ff8f563a)

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

KIM Queries

Modify the LAMMPS example to use a KIM query:

```
kim init EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
boundary p p p
variable a0 equals 4.05
lattice fcc ${a0}
region simbox block 0 1 0 1 0 1 units lattice
create_box 1 simbox
create_atoms 1 box
mass 1 1.0
kim interactions Al
run 0
```



```
kim init EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
boundary p p p
kim query a0 get_lattice_constant_cubic crystal=[fcc] species=[Al] \
                                         units=[angstrom]

lattice fcc ${a0}
region simbox block 0 1 0 1 0 1 units lattice
create_box 1 simbox
create_atoms 1 box
mass 1 1.0
kim interactions Al
run 0
```

See <https://openkim.org/doc/usage/kim-query/> for available queries.

Many other capabilities, see: https://docs.lammps.org/kim_commands.html

NEW FEATURE: Potential Citation Panel on Model Pages

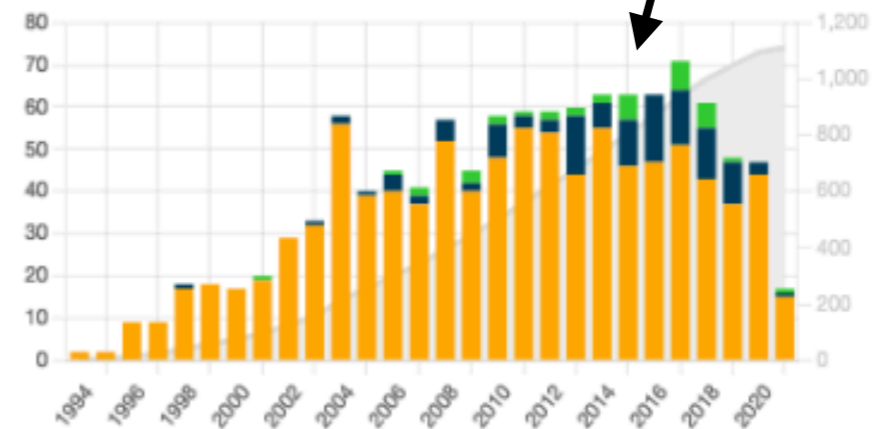
✓ EAM_Dynamo_ErcolessiAdams_1994_AI_MO_123629422045_005

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 ⓘ



Citations per year for potential broken into used/not used/unknown.

Word cloud based papers that used the potential

Papers citing the potential

1112 Citations (37 used)

★ Show Model Used Show All

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

- ★ H. Chabba and D. Dafir, "Atomistic Simulation Study of Mechanical Deformation of Al-Mg-Si Alloys," *International Journal of Engineering Research in Africa*. 2021. [link](#) Times cited: 0
Abstract: Aluminum alloys have been attracting significant attention. ... [read more](#)
- ★ A. L. Cazalilla, "Molecular dynamics simulation of ripple formation and propagation." 2019. [link](#) Times cited: 0
Abstract: Low and medium energy ion irradiation can induce different s... [read more](#)
- ⓘ P. Nyawere, "Parameterized Empirical Potentials For BaF 2 From Ab-Initio Methods Applied To The Study Of Superionic Transition Of C-BaF 2." 2018. [link](#) Times cited: 0

If you know if a paper used the potential, let us know!

KIM Community Building



OpenKIM in collaboration with the Materials Project established a central discussion forum for computational materials science at <https://matsci.org>



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KIM REVIEW

Commentaries on important peer-reviewed articles related to classical molecular simulations.

- Co-edited by Steve Plimpton + Advisory Board
- Discussion thread attached to each commentary on matsci.org
- Launch Fall 2021

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- Launch Fall 2021



Monthly webinar with the molecular simulation community

- Guest interviews
- KIM REVIEW spotlights
- OpenKIM features and demos
- Public Q&A
- Launch Fall 2021

KIM Coming Attractions

Symbol [units]	a_0	C_{11}	C_{12}	C_{44}	γ_{111}	γ_{100}	γ_{110}	γ_{112}
EAM-EA	-0.42	9.06	9.89	20.98	-35.43	-21.39	-18.41	-20.57
EAM-JNP	-1.51	2.96	50.4	51.08	-32.59	-19.14	-17.67	-46.19
EAM-MKB	-0.1	1.76	8.37	6.92	-68.25	-58.57	-54.22	36.5
EAM-MFM	0.02	5.08	8.66	4.46	-35.43	-21.27	-20.82	3.9
EAM-SL	0.02	-12.76	20.23	39.15	-54.16	-43.25	-41.9	-38.89
EAM-WKG	-0.59	5.18	9.03	3.44	-35.02	-23.88	-17.63	11.17
EAM-Z	-0.42	-2.9	23.4	44.85	-45.61	-32.03	-29.81	-33.87
EAM-ZWJ	0.82	17.5	43.7	20.2	-38.35	-27.83	-24.93	-41.09
EAM-ZM	0.02	7.95	6.2	3.97	-55.39	-49.34	-37.61	-7.07
EMT-JSN	-1.33	-50.1	-41.2	20.23	-47.57	-39.09	-44.34	-42.62
Morse-GW	-0.42	-24	6.48	108.26	113.08	129.84	125.73	-23.11
MEAM-JGH	0.02	2.13	7.6	-6.89	-44.21	-9.2	-10.59	80.3
MEAM-PF	0.02	4.9	8.78	48.75	-46.71	-18.5	-11.6	89.9
SMTBQ-SPA	-0.05	-13.5	32.9	23.41	-43.37	-30.72	-29.29	-57.19

Consumer Reports style Tool for IP Selection

- Select properties for comparison
- Define “loss function” (weights for properties)
- Plot error (loss) versus computational time

Karls, Bierbaum, Alemi, Elliott, Sethna, Tadmor, *J. Chem. Phys.*, 153:064104 (2020)

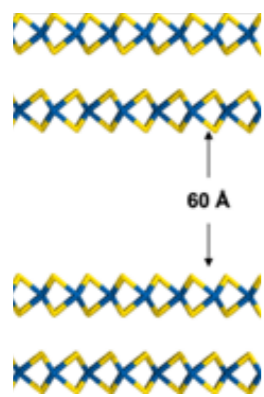
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MEAM-JGH	0.02	2.13	7.6	-6.89	-44.21	-9.2	-10.59	80.3
MEAM-PF	0.02	4.9	8.78	48.75	-46.71	-18.5	-11.6	89.9
SMTBQ-SPA	-0.05	-13.5	32.9	23.41	-43.37	-30.72	-29.29	-57.19

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Karls, Bierbaum, Alemi, Elliott, Sethna, Tadmor, *J. Chem. Phys.*, 153:064104 (2020)



MoS2 cleavage energy



Cyberloop for Accelerated Bionanomaterials Design

- Comparison of bonded force fields and reactive interatomic potentials
- Nanomaterials Modeler in CHARMM GUI

<https://www.charmm-gui.org/>

Choi et al., submitted (2021)

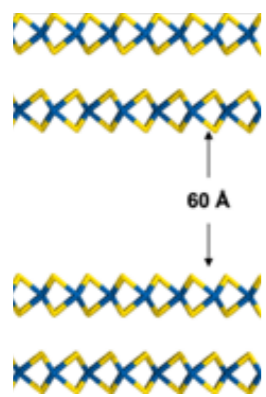
KIM Coming Attractions

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EAM-ZWJ	0.82	17.5	43.7	20.2	-38.35	-27.83	-24.93	-41.09
EAM-ZM	0.02	7.95	6.2	3.97	-55.39	-49.34	-37.61	-7.07
EMT-JSN	-1.33	-50.1	-41.2	20.23	-47.57	-39.09	-44.34	-42.62
Morse-GV	-0.42	-24	6.48	108.26	113.08	129.84	125.73	-23.11
MEAM-JGH	0.02	2.13	7.6	-6.89	-44.21	-9.2	-10.59	80.3
MEAM-PF	0.02	4.9	8.78	48.75	-46.71	-18.5	-11.6	89.9
SMTBQ-SPA	-0.05	-13.5	32.9	23.41	-43.37	-30.72	-29.29	-57.19

Consumer Reports style Tool for IP Selection

- Select properties for comparison
- Define “loss function” (weights for properties)
- Plot error (loss) versus computational time

Karls, Bierbaum, Alemi, Elliott, Sethna, Tadmor, *J. Chem. Phys.*, 153:064104 (2020)



MoS2 cleavage energy

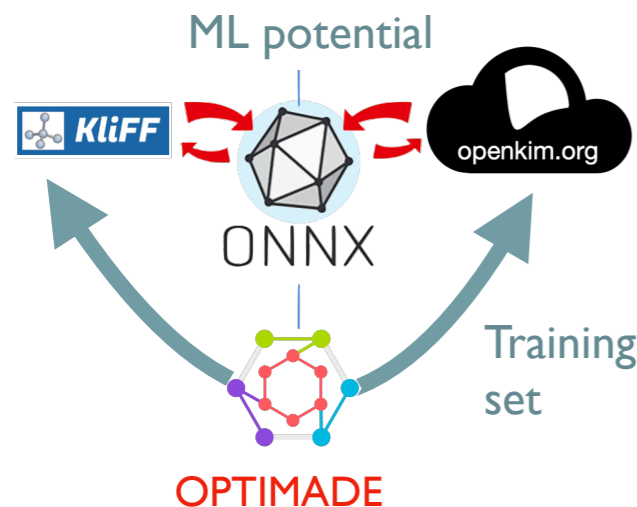


Cyberloop for Accelerated Bionanomaterials Design

- Comparison of bonded force fields and reactive interatomic potentials
- Nanomaterials Modeler in CHARMM GUI

<https://www.charmm-gui.org/>

Choi et al., submitted (2021)



ColabFit Framework (<https://colabfit.org>)

- KLIF Python-based Interatomic potential fitting framework
<https://github.com/openkim/kliff>
- Archiving of training sets
- Portable machine learning (ML) potentials

Stay informed...

OpenKIM · Knowledgebase of Interatomic Potentials

Getting Started About Citing Download/Upload Browse Support **Member Login**

Welcome to the Open Knowledgebase of Interatomic Models!

OpenKIM is a curated repository of interatomic potentials (IPs) and online framework for making classical molecular simulations of materials reliable, reproducible, and efficient. IPs archived in OpenKIM are verified for coding integrity, tested by computing their predictions for a variety of material properties, and issued DOIs for citation purposes. IPs downloaded from OpenKIM (as source or binary) work seamlessly with major simulation codes that conform to the KIM API standard. IP information and predictions are accessible via RESTful web queries and can be integrated in user simulation workflows. Content on OpenKIM is open source and freely available. OpenKIM is funded by the NSF.

- 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 parameters
kim_init SW_StillingerWeber_1985_Si_MO_405512
kim_query a0 get_lattice_constant_cubic crystal
# Setup diamond crystal
p p p
boundary
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.

Please cite the KIM Project and content obtained from this site if you use it in published work.

Models Tests [Contribute a Model](#)

Models

Click on an element to find interatomic models for that species. You can narrow the selection to models that support multiple species after you click.

H	Sp																		He
Li	Be										B	C	N	O	F				Ne
Na	Mg										Al	Si	P	S	Cl				Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br			Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I			Xe
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At			Rn
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	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

- ← Sign up to become a member
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 - free
 - few messages

Email us with any questions or requests:

- support@openkim.org

We're recruiting participants for a usability study of openkim.org.

- If interested, email me: tadmor@umn.edu

Check out the KIM Tutorial:

- “Getting Things Done using OpenKIM in LAMMPS”
- Friday 12:50 PM EDT