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)

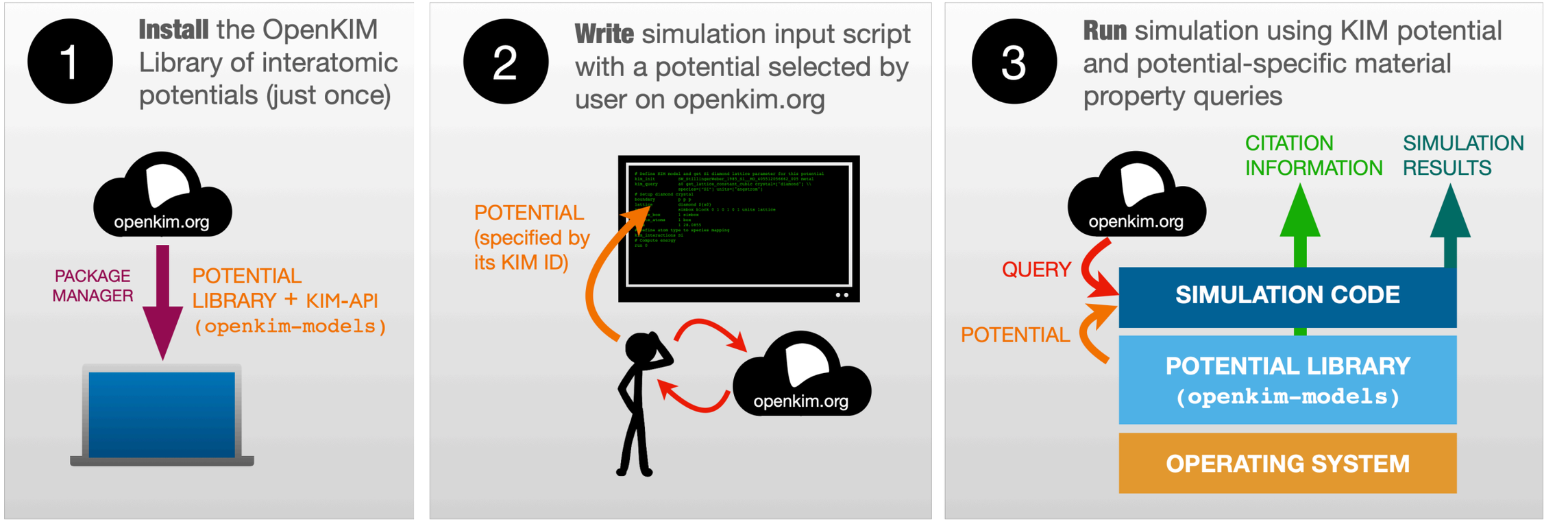
Core Developers

- 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

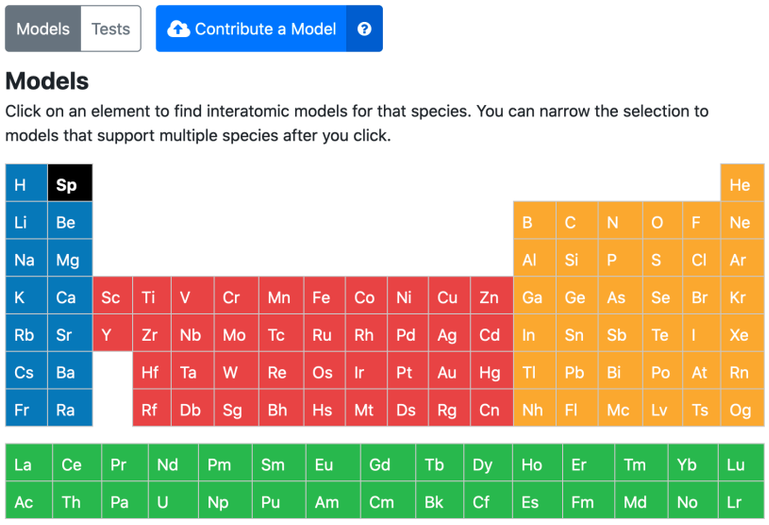
NSF CMMT (2019-)

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



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 kimpy openkim-models
```

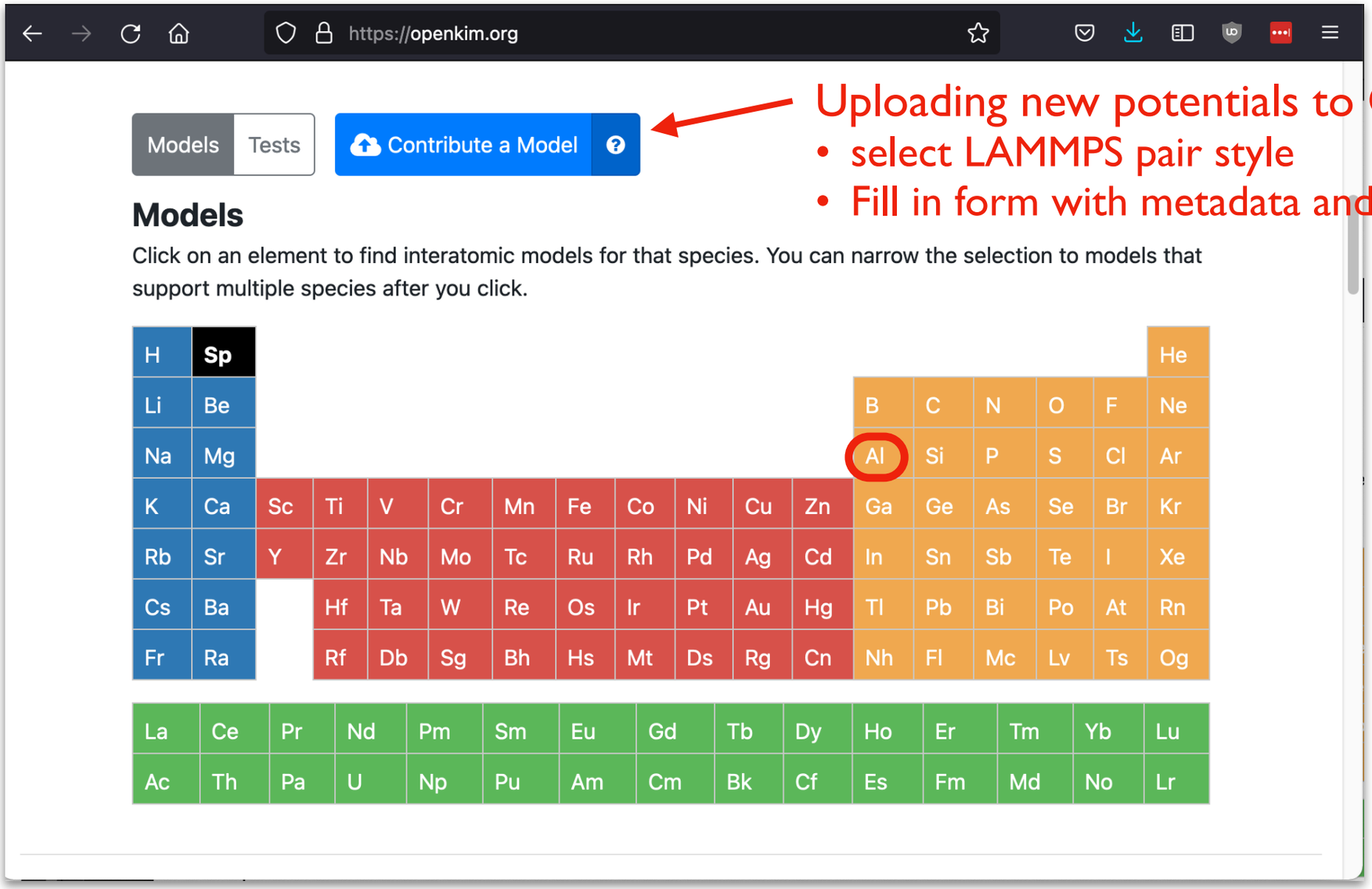
Similar procedures for openSUSE, Fedora, FreeBSD, AUR, CentOS, Debian, … soon for Windows.
See https://openkim.org/doc/usage/obtaining-models

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

Select an OpenKIM Potential



Uploading new potentials to OpenKIM is easy:

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

Select an OpenKIM Potential

https://openkim.org

Models | Tests

Contribute a Model

Uploading new potentials to OpenKIM is easy:

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

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																
Li	Be																
Na	Mg																
K	Ca	Sc	Ti	V													
Rb	Sr	Y	Zr	Nb													
Cs	Ba		Hf	Ta													
Fr	Ra		Rf	Db													

La	Ce	Pr	Nd	
Ac	Th	Pa	U	

OpenKIM — Getting Started | About | Citing | Download/Upload | Browse | Support | Member Login

- Model Drivers
- Models
- Test Drivers
- Tests
- Verification Checks
- Reference Data
- Developers

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 that support multiple species.

Narrow selection for multiple species (if desired)

Narrow species selection:

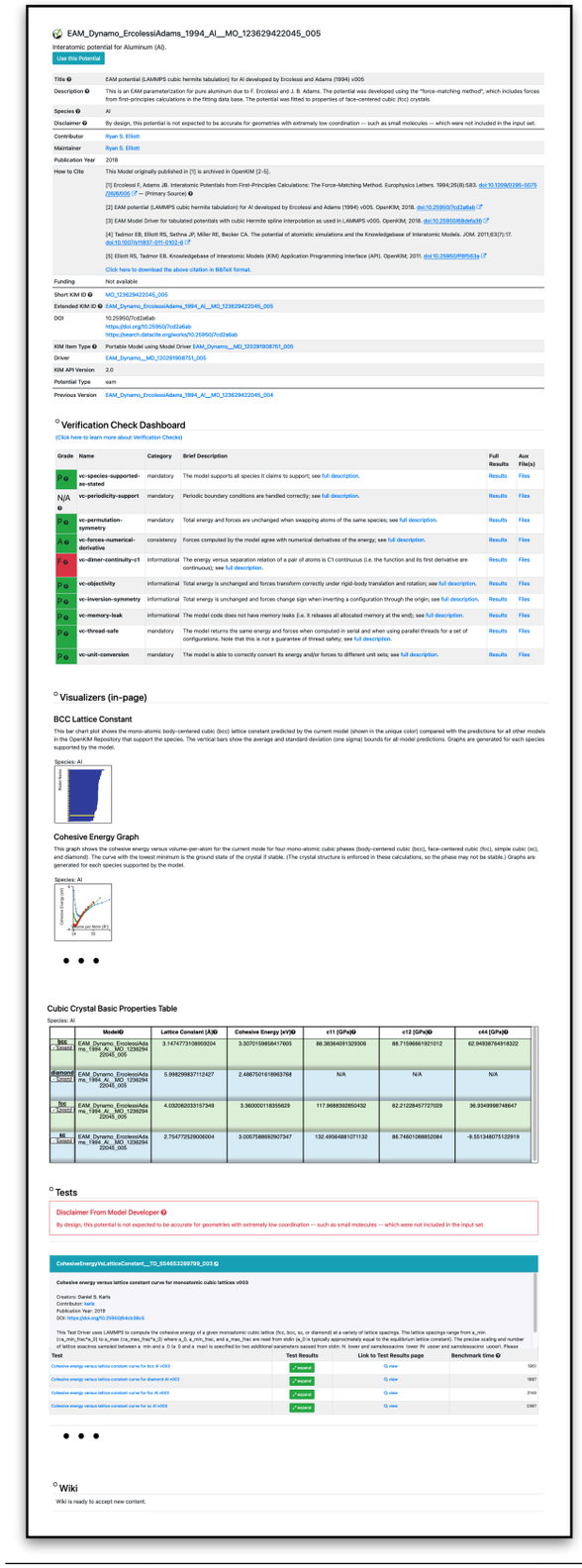
× Al

Begin typing to select species to narrow the selection; multiple species may be selected.

Al

Extended KIM ID	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_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

Select an OpenKIM Potential



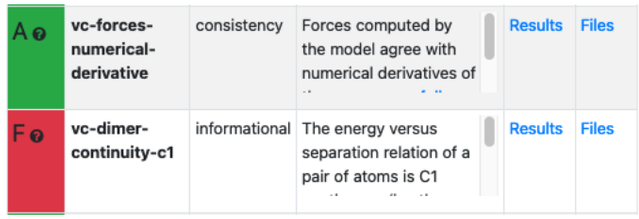
← KIM ID EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005

Metadata:

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

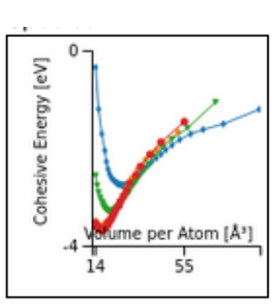
Verification Check (VC) dashboard

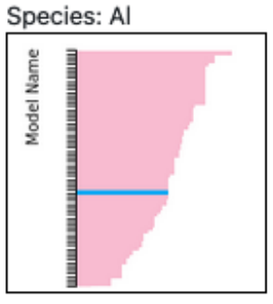
- Pass/fail or A-F grades on various VCs
- force numerical derivative, continuity, memory leaks, …



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
```

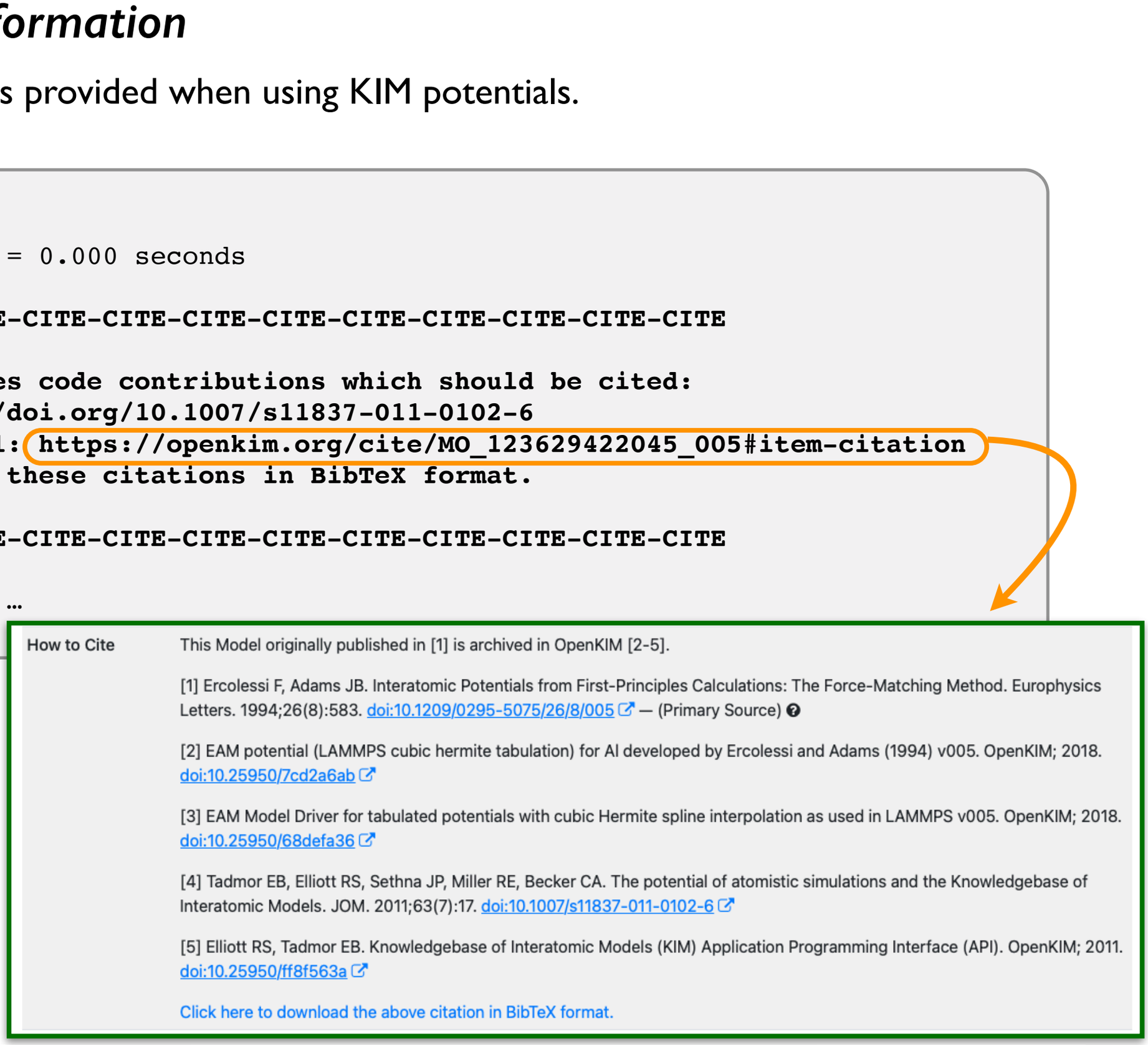
Only modifications needed to run with OpenKIM potential

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-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-CITE

Neighbor list info …
…
```

The **`log.lammps`** file contains all citations 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

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

Word cloud based papers that used the potential

Papers citing the potential

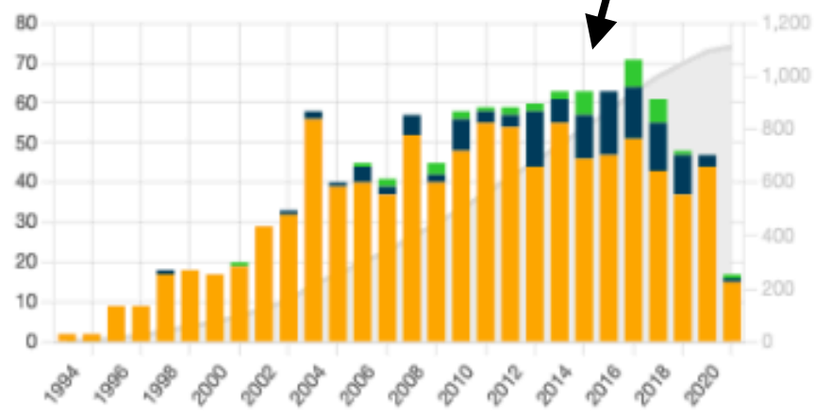
EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005

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



1112 Citations (37 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 💬 .

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

MATSCI COMMUNITY DISCOURSE

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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KIM Talk

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_{us}
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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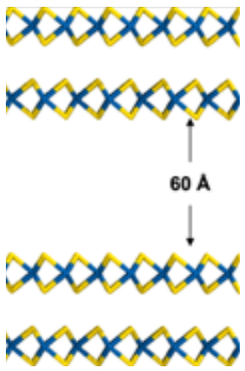

MoS2 cleavage energy

Cyberloop for Accelerated Bionanomaterials Design

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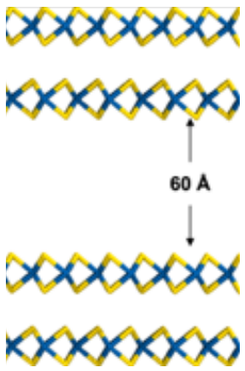

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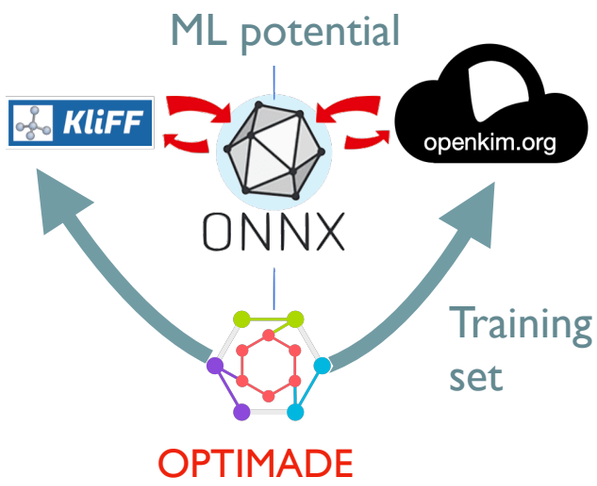
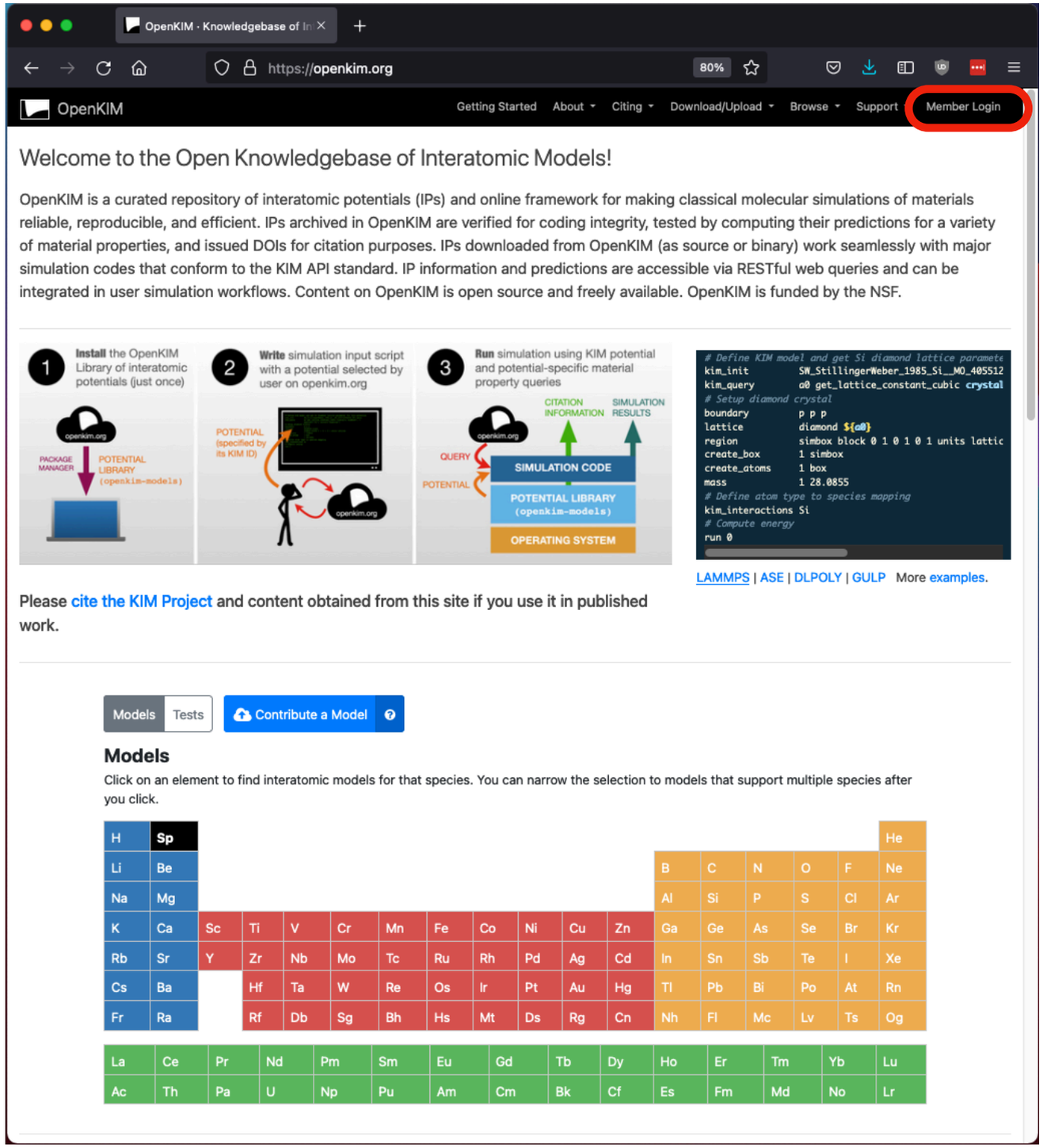


ColabFit Framework (https://colabfit.org)

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

Stay informed…



← Sign up to become a member

- https://openkim.org/member-login
- 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