Knowledgebase of Interatomic Models

http://OpenKIM.org

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Four Barriers faced by Molecular Modelers

Difficulties developers and users of interatomic models face include:

1. No easy access to an extensive list of reliable *reference data* from experiments and first principles calculations for fitting.

2. No easy access to implementations of existing models with known *provenance* and *cross-language capability*.

3. No *standardized tests* for evaluating properties of molecular systems.

4. No framework for evaluating the *precision and transferability* of models and therefore no *rigorous guidelines* for choosing an appropriate model for a given application.

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Knowledgebase of Interatomic Models (KIM)

The Knowledgebase of Interatomic Models (KIM) project is based on a four-year NSF cyber-enabled discovery and innovation (CDI) grant and has the following main objectives:

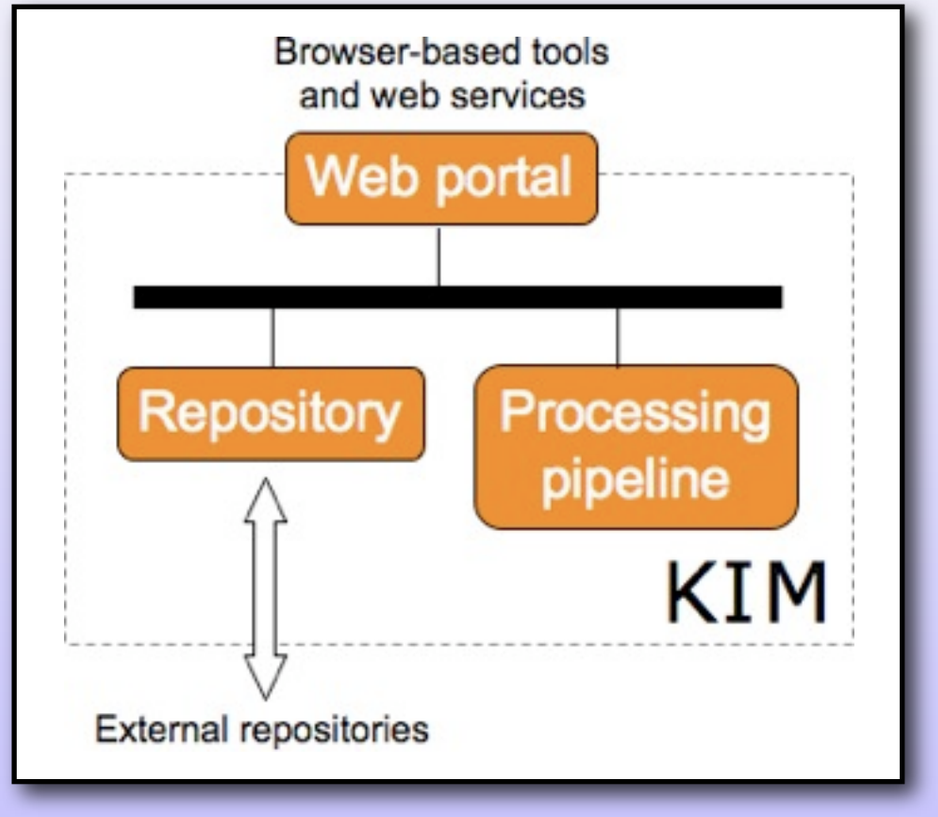
Stage I

- Development of an online open resource for *standardized testing* long-term *warehousing* of interatomic models (potentials and force fields) and data.
- Development of an *application programming interface (API)* standard for atomistic simulations, which will allow any interatomic model to work seamlessly with any atomistic simulation code.

Stage II

- Fostering the development of a quantitative *theory of transferability* of interatomic models to provide *guidance for selecting* application-appropriate models based on rigorous criteria, and *error bounds* on results.

KIM Overview



Repository: A user-extendible database of

- interatomic *Models*
- standardized *Tests* (simulation codes)
- *Predictions* (results from Model-Test couplings)
- *Reference Data* (obtained from experiments and first principles calculations)

Web portal: A web interface that will facilitate:

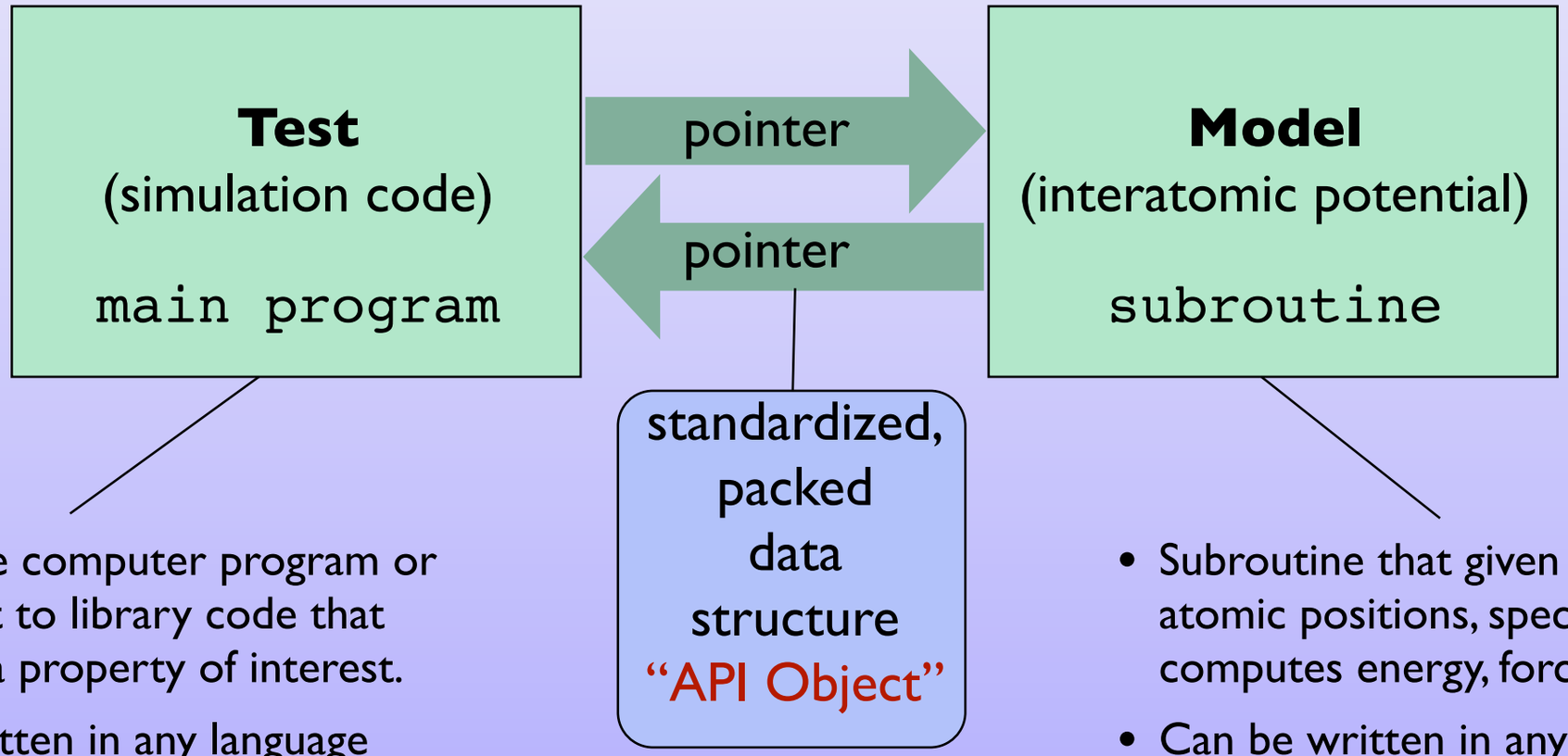
- user upload and download of Tests, Models and Reference Data
- searching and querying the repository
- comparing and visualizing Predictions and Reference Data
- recording user feedback

Processing pipeline: An automatic system for generating *Predictions* by mating *Tests* and *Models* in the KIM Repository.

- puts the "knowledge" in "knowledgebase"

KIM API Standard

An Application Programming Interface (API) standard has been defined which enables any Test to work seamlessly with any Model.



- Stand-alone computer program or input script to library code that computes a property of interest.
- Can be written in any language supported by the API (Fortran 77, Fortran 90, C, C++, Python, Java, ...)

- Subroutine that given a set of atomic positions, species, ... computes energy, forces, ...
- Can be written in any language supported by the API (Fortran 77, Fortran 90, C, C++, Python, Java, ...)

Objective: to have the KIM API be adopted as a **community standard** so that <u>any</u> interatomic *Model* will be able to be run with <u>any</u> simulation code.

Web page demo of Models, Tests, and Drivers

"Essentially, all models are wrong, but some are useful."

— George E. P. Box

OpenKIM

Welcome to the Knowledgebase of Interatomic Models

An online resource for standardized testing and long-term warehousing of interatomic models and data. This includes the development of *application programming interface* (API) standards for coupling atomistic simulation codes and interatomic potential subroutines.

Please choose an item from the above menu.

Latest News

Visit the news archive for all news items

Contact us if you would like to contribute a news item.

Updated *pair_style kim* release in LAMMPS 3Aug13

26-Jul-2013

The KIM development team is please to announce the release of a openkim-api-v1.2.0 compatible version of the LAMMPS pair style kim. The version of pair_style kim is available in the August 3th, 2013 version of lammps (lammps-3Aug13).

See more Updated pair_style kim release in LAMMPS 3Aug13

KIM API version 1.2.0 released

12-Jul-2013

The KIM development team is pleased to announce the release of version 1.2.0 of the KIM application programming interface (API). By conforming to this API, an atomistic simulation code will seamlessly work with any KIM-compliant interatomic model written in any supported language. This release includes a completely redesigned Make system with many new features and benefits, a new NEIGH_RVEC_H NBC, a streamlined scheme for specifying a Model (or Model Driver name) and its associated "model_init()" function name, other minor changes to the api, bug fixes, portability improvements, and some new examples.

See more KIM API version 1.2.0 released

KIM Content Carnival in Singapore (October 9-12, 2012)

20-Jul-2012

Come to Singapore this fall during October 9-12, 2012 for a 4-day free event, to learn about KIM and make your potential compatible with the KIM Application Programming Interface (API).

See more KIM Content Carnival in Singapore (October 9-12, 2012)

KIM API version 1.1.0 released

12-Jul-2012

The KIM development team is pleased to announce the release of version 1.1.0 of the KIM application programming interface (API). By conforming to this API, an atomistic simulation code will seamlessly work with any KIM-compliant interatomic model written in any supported language. This release includes many bug fixes, portability improvements, an updated Model Driver interface, and some minor changes to functionality.

See more KIM API version 1.1.0 released

KIM Content Carnival in Aachen, Germany (August 20-23, 2012)

21-May-2012

Come to Aachen, Germany this summer during August 20-23, 2012 for a 4-day free event, to learn about KIM and make your potential compatible with the KIM Application Programming Interface (API).

See more KIM Content Carnival in Aachen, Germany (August 20-23, 2012)

KIM Board Election Results

07-Feb-2012

The slate of nominees for the KIM Board (Ronald Miller, Sadasivan Shankar and Aidan Thompson) suggested by the Nominating Committe has been *unanimously* approved by the KIM Membership.

See more KIM Board Election Results

KIM Requirements Document Launched

20-Sep-2011

The KIM development team is pleased to announce that the KIM Requirements Document (RD) is now available online here. RDs are common in industry where they are used to fully define all aspects of new products during the development stage. The KIM RD addresses topics ranging from the organization and governance of KIM to the details of the KIM application programming interface (API).

See more KIM Requirements Document Launched

Article on KIM published in JOM

30-Jul-2011

A feature article titled "The Potential of Atomistic Simulations and the Knowledgebase of Interatomic Models" has recently been published in the July issue of *JOM*, the member journal of TMS. The article describes the main objectives of the KIM project and its status as of July 2011.

See more Article on KIM published in JOM

KIM Inaugural Meeting held in San Diego

01-Mar-2011

The KIM project had its Inaugural Meeting in San Diego, CA, on February 26-27, 2011. Important steps were taken at this meeting to define the goals and structure of KIM based on the needs of the atomistic simulation community.

See more KIM Inaugural Meeting held in San Diego

Job Openings

Contact us if you would like to post a job related to interatomic model development.

Excellent Junior and Senior Researchers Needed for KIM Development

20-May-2012

The Knowledgebase of Interatomic Models (KIM) project is seeking excellent researchers at both junior and senior levels with strong computational skills to work on various aspects of KIM development.

See more here

The OpenKIM project is supported by NSF funding.

KIM Application Programming Interface (API)

Overview

The KIM API is an Application Programming Interface for atomistic simulations. The API provides a standard for exchanging information between atomistic simulation codes (molecular dynamics, molecular statics, lattice dynamics, Monte Carlo, etc.) and interatomic models (potentials or force fields). It also includes a set of library routines for using the API with bindings for

- FORTRAN 77
- Fortran 90/95
- C
- C++

By conforming to this API, an atomistic simulation code will seamlessly work with any KIM-compliant interatomic model written in any supported language. The interface is computationally efficient and often requires relatively minor changes to existing codes.

Downloading the Most Recent API Package

The most recent packaged download of the KIM API is available here:

openkim-api-latest

Details about the latest release and installation instructions are available here.

Our API is under version control with Git hosted at GitHub.

Archive of Older Versions:

- openkim-api-v1.2.1.tgz - first available on 2013/07/21
- openkim-api-v1.2.0.tgz - first available on 2013/07/12
- openkim-api-v1.1.1.tgz - first available on 2012/08/19
- openkim-api-v1.1.0.tgz - first available on 2012/07/12
- openkim-api-v1.0.1.tgz - first available on 2012/02/25
- openkim-api-v1.0.0.tgz - first available on 2011/02/22
- openkim-api-v0.2.0.tgz - first available on 2011/09/15
- openkim-api-v0.1.2.tgz - first available on 2011/08/22
- openkim-api-v0.1.1.tgz - first available on 2011/08/16
- openkim-api-v0.1.0.tgz - first available on 2011/08/08

What is in the api package?

The current version of the openkim-api package includes the api itself and the following example codes:

Models:

(for more information see the file ${KD}/EXAMPLES/MODELS/EXAMPLES.README)

- Lennard-Jones pair potential shifted to zero energy at cutoff.
  - Parameterized for Ar and Ne (ex_model_Ar_P_LJ, ex_model_Ne_P_LJ)
  - An implementation for Ne that is optimized for computational speed (ex_model_Ne_P_fastLJ)
  - An implementation for Ne that demonstrates the use of F77 with the api (ex_model_Ne_P_LJ_NEIGH_PURE_H)
- Lennard-Jones pair potential with quadratic cutoff function.
  - Parameterized for Ar and Ne. (ex_model_Ar_P_MLJ_C, ex_model_Ar_P_MLJ_CLUSTER_C, ex_model_Ar_P_MLJ_CLUSTER_F90, ex_model_Ar_P_MLJ_F90, ex_model_Ar_P_MLJ_MI_OPBC_H_F, ex_model_Ar_P_MLJ_NEIGH_PURE_H_F, ex_model_Ar_MLJ_NEIGH_RVEC_F, ex_model_Ne_P_MLJ_NEIGH_RVEC_H)
  - Note: multiple versions of this potential are provided in order to demonstrate the various features and options of the api.
- Morse pair potential shifted to zero energy at cutoff.
  - Parameterized for Ar and Ne (ex_model_Ar_P_Morse, ex_model_Ne_P_Morse)
- Lennard-Jones alloy pair potential with quadratic cutoff function.
  - Parameterized for ArNe alloys (ex_model_ArNe_P_MLJ_NEIGH_RVEC_F)
- Ercolessi Adams EAM potential for Al.
- Johnson EAM potential for Cu.

Tests:

(for more information see the file ${KD}/EXAMPLES/TESTS/EXAMPLES.README)

- Compute the energy and forces on a finite chunk of an fcc crystal. Versions for Al, Ar, Cu and Ne are provided. (ex_test_Al_free_cluster, ex_test_Ar_free_cluster, ex_test_Ar_free_cluster_CLUSTER_C, ex_test_Ar_free_cluster_CLUSTER_F90, ex_test_Ar_free_cluster_CLUSTER_memory_F90, ex_text_Cu_free_cluster, ex_test_Ne_free_cluster, ex_test_Ne_free_cluster_SI, ex_test_Ne_free_cluster_stiff)
  - The ex_test_Ne_free_cluster_SI and ex_test_Ne_free_cluster_stiff versions use the SI unit system and compute the Hessian for the cluster, respectively.
- Compute the relaxed lattice spacing and cohesive energy of a periodic infinite fcc crystal of Al, Ar, and Ne. (ex_test_Al_FCCcohesive_MI_OPBC, ex_test_Ar_FCCcohesive_MI_OPBC, ex_test_Ar_FCCcohesive_NEIGH_PURE, ex_test_Ar_FCCcohesive_NEIGH_RVEC)
- Compute the relaxed lattice spacing and cohesive energy of a periodic infinite B2 crystal of ArNe. (ex_test_ArNe_periodic_B2_NEIGH_RVEC)
- Compute the relaxed lattice spacing and cohesive energy of a periodic infinite fcc crystal of Ar for a variety of Model cutoff values. (ex_test_Ar_FCCcoheisveCutoff_NEIGH_RVEC)
- Compute energy and forces for two models in one Test (ex_test_Ar_multiple_models) This Test is meant to illustrate some more advanced usage of the api.

Verification Checks:

- Perform a smart numerical derivative of the energy and compare the results to the forces. (vc_forces_numer_deriv)
- Perform a different smart numerical derivative of the energy and compare the results to the forces. (vc_forces_delta)
- Perform an energy and forces computation for a provided configuration and compare the results to a provided expected result (vc_config_ener_forces)

KIM API Boot Camp: Learning to use the API

Although the below Boot Camp inforamtion is for openkim-api-v1.0.0/v1.1.0, much of the inforamtion is still valid and useful. The API is not difficult to use but involves new concepts and requires some training. For users interested in adapting their programs (simulation codes and/or interatomic models) to become "KIM compliant" (i.e. conform to the KIM API), we recommend the following training:

1. Dowload the following presentations and training material that will referred to and used by the online lectures described below.
   - KIM Overview Talk by Prof. Ellad B. Tadmor (pdf file)
   - Introduction to the KIM API by Prof. Ryan S. Elliott (pdf file)
   - Training material (v1.0.0 gzipped tarball) or (v1.1.0 gzipped tarball)

   NOTE: The resources listed above may also be downloaded as a single package here.

   Unpack the training material tarball using the following Unix/Linux command:

   ```
   % tar zxvf openkim-api-training-v1.0.0.tgz
   ```

   This package contains the following example files:

   ```
   openkim-api-training-v1.0.0/MODELs/ex_model_Ar_P_Morse_01C/
   openkim-api-training-v1.0.0/MODELs/ex_model_Ar_P_Morse_02C/
   ...
   openkim-api-training-v1.0.0/MODELs/ex_model_Ar_P_Morse_14C/
   ```

   Each of these examples is incrementally more complex than the previous one. It's a great way to develop an understanding of the API. The online lectures described below go over these examples in a step-by-step fashion.

2. Watch the following online lectures:
   - **Overview of the KIM Project by Prof. Ellad B. Tadmor**.... VIEW LECTURE
     - Motivation for the KIM project and its goals
     - Basic openKIM.org components (Data, Models, Tests)
     - Processing pipeline and the KIM API
     - Examples of how openKIM.org will work in practice
   - **Introduction to the KIM API by Prof. Ryan S. Elliott – Part I**.... VIEW LECTURE
     - Overview of the KIM API
     - Basic Model components, optional computation, process_ mechanisms
     - Walk through of Examples 01-04
       - CLUSTER energy
       - CLUSTER energy, force, particleEnergy (all optional)
       - CLUSTER virial, particleVirial, hessian
       - CLUSTER process_dEdr, process_d2Edr2
   - **Introduction to the KIM API by Prof. Ryan S. Elliott – Part II**.... VIEW LECTURE
     - Neighbor lists and boundary conditions (NBCs), half lists, iterator/locator modes
     - Walk through of Examples 04-06
       - Review of Example 04, NBC CLUSTER energy, force, ...
       - NBC NEIGH_PURE_H
       - Iterator mode
   - **Introduction to the KIM API by Prof. Ryan S. Elliott – Part III**.... VIEW LECTURE
     - Walk through of Examples 07-08
       - Full neighbor lists
       - Parallel computing
       - NBC NEIGH_PURE_F
       - NBC NEIGH_RVEC_F
     - How Tests provide neighbor lists (ex_test_Ar_FCCcohesive_NEIGH_PURE)
   - **Introduction to the KIM API by Prof. Ryan S. Elliott – Part IV**.... VIEW LECTURE
     - Walk through of Examples 09-11
       - NBCs MI_OPBC_H and MI_OPBC_F
       - Model Parameters
       - Flexible unit handling

3. Do the "Boot Camp" exercises given in this assignment: bootcamp_exercises.pdf

   Compare your results with the solutions in bootcamp_exercises_SOLUTION.pdf.

   The exercises involve simulations using a basic KIM-compliant molecular statics/molecular dynamics code called "MiniMol" which can be obtained here: MiniMol Program (v1.0.0 gzipped tarball) or (v1.1.1 gzipped tarball)

   To run this program you must first install the KIM API (see "Downloading the Most Recent API Package" above). Then do the following:

   ```
   % mv MiniMol.tgz $KIM_DIR/TESTs
   % cd $KIM_DIR/Tests
   % tar zxvf MiniMol.tgz
   % cd $KIM_DIR
   % make
   % rehash  # you only need to do this if you are using csh or tcsh
   ```

   In the above, "$KIM_DIR" is the directory where you installed the openKIM API package. This will create the executable MiniMol in $KIM_DIR/TESTs/MiniMol.

   All of the data files needed for the Boot Camp exercises are stored in $KIM_DIR/TESTs/MiniMol/Data

4. Read the "README" file in the DOCs directory of the KIM API distribution package:

   $KIM_DIR/DOCs/README

   Here "$KIM_DIR" represents the directory where you installed the KIM API. The README file walks you through the examples provided with the API distribution and directs you to other documentation files that you should read.

With the above training completed, a user should be ready to adapt existing code to become KIM compliant and to write new KIM compliant code from scratch.

To test your understanding of this process, you can try the following exercise. Take a simple stand-alone program that reads a file with atom types and coordinates and, treating this as an isolated cluster of atoms, computes the system's energy and the energy and force components for each atom. Your task is to transform this program into two parts: A KIM compliant Model (kcc_model_exp6) and a KIM compliant Test (kcc_test_cluster). The example codes (in C and Fortran 90) can be downloaded here:

- KCC_Hands-on_C.tgz
- KCC_Hands-on_F90.tgz

Getting Help

Support is always available by sending an email with a question and all relevant information to

openkim@googlegroups.com

The message will be posted to the openkim google group:

http://groups.google.com/group/openkim

Members of the openKIM development team actively monitor this forum and will do their best to respond to questions in a timely fashion. This forum is also used to announce minor new releases and bug fixes.

It is highly recommended for users who plan to work with the KIM API to become members of the openkim group. (Just go to the above link and click on "Join this group" on the right of the screen.)

pair_style kim command

Syntax:

```
pair_style kim virialmode model
```

- virialmode = KIMvirial or LAMMPSvirial
- model = name of KIM model (potential)

Examples:

```
pair_style kim KIMvirial model_Ar_P_Morse
pair_coeff * * Ar Ar
```

Description:

This pair style is a wrapper on the Knowledge Base for Interatomic Models (KIM) repository of interatomic potentials, so that they can be used by LAMMPS scripts.

In KIM lingo, a potential is a "model" and a model contains both the analytic formulas that define the potential as well as the parameters needed to run it for one or more materials, including coefficients and cutoffs.

The argument *virialmode* determines how the global virial is calculated. If *KIMvirial* is specified, the KIM model performs the global virial calculation. If *LAMMPSvirial* is specified, LAMMPS computes the global virial using its fdotr mechanism.

The argument *model* is the name of the KIM model for a specific potential as KIM defines it. In principle, LAMMPS can invoke any KIM model. You should get an error or warning message from either LAMMPS or KIM if there is an incompatibility.

Only a single pair_coeff command is used with the *kim* style which specifies the mapping of LAMMPS atom types to KIM elements. This is done by specifying N additional arguments after the * * in the pair_coeff command, where N is the number of LAMMPS atom types:

- N element names = mapping of KIM elements to atom types

As an example, imagine the KIM model supports Si and C atoms. If your LAMMPS simulation has 4 atom types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to Si as defined within KIM. The final C argument maps LAMMPS atom type 4 to C as defined within KIM. If a mapping value is specified as NULL, the mapping is not performed. This can only be used when a *kim* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

In addition to the usual LAMMPS error messages, the KIM library itself may generate errors, which should be printed to the screen. In this case it is also useful to check the kim.log file for additional error information. This file kim.log should be generated in the same directory where LAMMPS is running.

Here is information on how to build KIM for use with LAMMPS. There is a directory src/KIM/ with an important file in it: Makefile.lammps. When you do 'make yes-kim' LAMMPS will use the settings in src/KIM/Makefile.lammps to find KIM header files and the KIM library itself for linking purposes. Thus, you should ensure Makefile.lammps has the correct settings for your system and your build of KIM.

Consult the KIM documentation for further details on KIM specifics.

OpenKIM is available for download from this site, namely http://openkim.org. The tarball you download is "openkim-api-vX.X.X.tgz", which can be unpacked via

```
tar xvfz openkim*tgz
```

The openkim-api-vX.X.X/DOCS directory has further documentation. For more information on installing KIM and troubleshooting refer to openkim/INSTALL.

Here is a brief summary of how to build KIM:

1. If you have previously used the openkim-api package (versions 1.1.1 or below), it is recommended that you remove all associated environment variables from your environment. (These include, KIM_DIR, KIM_INTEL, KIM_SYSTEM32, KIM_DYNAMIC, KIM_API_DIR, KIM_TESTS_DIR, KIM_MODEL_DRIVERS_DIR, and KIM_MODELS_DIR.) All setting are now specified in the Makefile.KIM_Config file.
2. Set up the Makefile.KIM_Config file

```
(a) Copy the file Makefile.KIM_Config.example to Makefile.KIM_Config
    For example, if you untarred the `openkim-api-vX.X.X.tgz' tarball in
    your home directory, you would do:

    % cd $HOME/openkim-api-vX.X.X
    % cp Makefile.KIM_Config.example Makefile.KIM_Config

    The `%' symbol represents the bash sell prompt and should not be typed.


    (Above `vX.X.X' represents the current release number.)

(b) Edit the file Makefile.KIM_Config and set the appropriate value for the
    KIM_DIR variable.  This must expand to an absolute path.  Using the same
    assumptions as above, this would be

    KIM_DIR = $(HOME)/openkim-api-vX.X.X

(c) If appropriate, set explicit values for the remaining three
    directories

    KIM_MODEL_DRIVERS_DIR =
    KIM_MODELS_DIR =
    KIM_TESTS_DIR =

    If these lines are commented out, defaults will be provided by the
    openkim-api make system.

(d) Set the value of KIM_COMPILERSUITE.  Possible values are `GCC' and
    `INTEL'.

    KIM_COMPILERSUITE = GCC

(e) Set the value of KIM_SYSTEMLINKER. Possible values are `linux',
    `freebsd', and `darwin'.

    KIM_SYSTEMLINKER = linux

(f) Set the value of KIM_SYSTEMARCH.  Possible values are `32bit' and
    `64bit'.

    KIM_SYSTEMARCH = 64bit

(g) Set the value of KIM_LINK.  Possible values are `dynamic-load',
    `dynamic-link', and `static-link'.

    KIM_LINK = dynamic-load

    `dynamic-load' is the preferred option. (Unless performance or
    other issues require it, you should use dynamic-load.)
    `dynamic-link' is like `dynamic-load' but does not use the dl.h
    library.  This option requires a more complicated Makefile
    process, but may improve computation time in some instances.
    `static-link' only works with ONE Model and AT MOST ONE Model
    Driver (in order to avoid the possibility of symbol
    clashes).

(h) Set override values for other variables, if necessary, by
    adding the desired variable name (after the "# overwrite
    default variable values here" line) and filling in appropriate
    values.

    # overwrite default variable values here

    # overwrite default compiler options

    CC =
    CXX =
    FC =

    # overwrite default compiler option flag lists
    FFLAGS   =
    CCFLAGS  =
    CXXFLAGS =
    LDFLAGS  =

    # overwrite default linker options
    LDSHAREDFLAG =
    LINKSONAME =
    LDWHOLEARCHIVESTARTFLAG =
    LDWHOLEARCHIVEENDFLAG =

    # overwrite default install directories
    package_name =
    prefix =
    libdir =
```

3. In the remainder of the documentation we will use the string $KD to represent the location of the openkim-api source package (the value of the KIM_DIR variable discussed above). If you wish to, type the below commands exactly as written to set the shell variable KD to the appropriate value:

```
bash:
% export KD=$HOME/openkim-api-vX.X.X
```

4. To compile the package, including the provided examples, change to the $KD directory and execute `make examples' and then `make':

```
% cd $KD
% make examples
% make

  This builds all Model Drivers, Models, Tests, and the openkim-api service
  routine library.  The targets defined by the Makefile in this directory
  include:

    `make'              -- compiles the API and all Models and Tests
    `make all'          -- same as `make'
    `make clean'        -- will remove appropriate .o, .mod, .a, .so and
                           executable files
    `make install'      -- install files to `/usr/local/lib' by default
    `make uninstall'    -- delete files installed by `make install'
    `make openkim-api'  -- compiles only the API
    `make examples'     -- copies examples into the appropriate
                           directories (no overwrite)
    `make examples-force' -- copies examples into the appropriate
                           directories (overwrite)
    `make examples-clean' -- remove all examples from the MODEL_DRIVERS,
                           MODELS, and TESTS directories.
```

5. Verify that the compilation was successful by running a Test.

```
The provided example Tests read in the name of a Model (or Models)
which they use to perform their calculations.  For most Tests the
name of the Model can be piped in using an `echo' command.  For
example, the following Fortran 90 Test reads in one Model:

% cd $KD/TESTs/test_Ar_free_cluster_CLUSTER_F90
% echo "model_Ar_P_MLJ_CLUSTER_C" | ./test_Ar_free_cluster_CLUSTER_F90

(See the README files in the Test directories for an explanation of what
the Tests do.)
```

6. Each Test (and Model) has its own make file for compiling and linking. If changes are made to the code, re-compile (from the $KD directory).

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since KIM stores the potential parameters. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the KIM package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This current version of pair_style kim is compatible with the openkim-api package version 1.2.0 and higher.

Related commands:

pair_coeff

Default: none

Models - by Model Drivers

Alphabetical By Species By Driver By Tests

CF_Tersoff__MD_941831228559_000

Title	Extended KIM ID
CF_T2_Si	CF_T2_Si__MO_128738412454_000
CF_T3_Si	CF_T3_Si__MO_101002579388_000

CF_exTersoff__MD_151418255940_000

Title	Extended KIM ID
CF_ELAST_Si	CF_ELAST_Si__MO_113514803518_000
CF_MELT_Si	CF_MELT_Si__MO_179316347627_000
CF_MOD_Si	CF_MOD_Si__MO_119804179894_000

EAM_Dynamo__MD_120291908751_000

Title	Extended KIM ID
EAM_Dynamo_Ackland_Bacon_Fe	EAM_Dynamo_Ackland_Bacon_Fe__MO_142799717516_000
EAM_Dynamo_Ackland_Mendelev_FeP	EAM_Dynamo_Ackland_Mendelev_FeP__MO_884343146310_000
EAM_Dynamo_Ackland_Ti	EAM_Dynamo_Ackland_Ti__MO_748534961139_000
EAM_Dynamo_Ackland_Tichy_Ag	EAM_Dynamo_Ackland_Tichy_Ag__MO_212700056563_000
EAM_Dynamo_Ackland_Tichy_Au	EAM_Dynamo_Ackland_Tichy_Au__MO_104891429740_000
EAM_Dynamo_Ackland_Tichy_Cu	EAM_Dynamo_Ackland_Tichy_Cu__MO_179025990738_000
EAM_Dynamo_Ackland_Tichy_Ni	EAM_Dynamo_Ackland_Tichy_Ni__MO_977363131043_000
EAM_Dynamo_Ackland_W	EAM_Dynamo_Ackland_W__MO_141627196590_000
EAM_Dynamo_Adams_Foiles_Ag_u4	EAM_Dynamo_Adams_Foiles_Ag_u4__MO_366710161005_000
EAM_Dynamo_Adams_Foiles_Au_u4	EAM_Dynamo_Adams_Foiles_Au_u4__MO_542075092223_000
EAM_Dynamo_Adams_Foiles_Cu_u4	EAM_Dynamo_Adams_Foiles_Cu_u4__MO_783346091107_000
EAM_Dynamo_Adams_Foiles_Ni_u4	EAM_Dynamo_Adams_Foiles_Ni_u4__MO_130989848973_000
EAM_Dynamo_Adams_Foiles_Pt_u4	EAM_Dynamo_Adams_Foiles_Pt_u4__MO_117515733772_000
EAM_Dynamo_Angelo_Moody_NiAlH	EAM_Dynamo_Angelo_Moody_NiAlH__MO_418978237058_000
EAM_Dynamo_Bonny_Pasianot_FeCuNi	EAM_Dynamo_Bonny_Pasianot_FeCuNi__MO_469343973171_000
EAM_Dynamo_Bonny_Pasianot_FeNi	EAM_Dynamo_Bonny_Pasianot_FeNi__MO_267721408934_000
EAM_Dynamo_Cai_Ye_AlCu	EAM_Dynamo_Cai_Ye_AlCu__MO_942551040047_000
EAM_Dynamo_Ercolessi_Adams_Al	EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000
EAM_Dynamo_Fellinger_Park_Nb	EAM_Dynamo_Fellinger_Park_Nb__MO_102133002179_000
EAM_Dynamo_Foiles_Cu_u3	EAM_Dynamo_Foiles_Cu_u3__MO_468316472729_000
EAM_Dynamo_Foiles_CuNi	EAM_Dynamo_Foiles_CuNi__MO_869958188303_000
EAM_Dynamo_Fortini_Mendelev_Ru	EAM_Dynamo_Fortini_Mendelev_Ru__MO_114077951467_000
EAM_Dynamo_Grochola_Russo_Au	EAM_Dynamo_Grochola_Russo_Au__MO_852752408985_000
EAM_Dynamo_Hepburn_Ackland_FeC	EAM_Dynamo_Hepburn_Ackland_FeC__MO_143977152728_000
EAM_Dynamo_Hoyt_Garvin_PbCu	EAM_Dynamo_Hoyt_Garvin_PbCu__MO_119135752160_000
EAM_Dynamo_Landa_Wynblatt_AlPb	EAM_Dynamo_Landa_Wynblatt_AlPb__MO_699137396381_000
EAM_Dynamo_Li_Siegel_Ta	EAM_Dynamo_Li_Siegel_Ta__MO_103054252769_000
EAM_Dynamo_Liu_Adams_MgAl	EAM_Dynamo_Liu_Adams_MgAl__MO_544273640230_000
EAM_Dynamo_Liu_Ercolessi_Al	EAM_Dynamo_Liu_Ercolessi_Al__MO_194915988663_000
EAM_Dynamo_Liu_Liu_AlCu	EAM_Dynamo_Liu_Liu_AlCu__MO_128706169020_000
EAM_Dynamo_Liu_Liu_AlFe	EAM_Dynamo_Liu_Liu_AlFe__MO_503784222035_000
EAM_Dynamo_Liu_Ohotnicky_MgAl	EAM_Dynamo_Liu_Ohotnicky_MgAl__MO_135676685253_000
EAM_Dynamo_Mendelev_Asta_AlMg	EAM_Dynamo_Mendelev_Asta_AlMg__MO_658278549784_000
EAM_Dynamo_Mendelev_Han_Fe_2	EAM_Dynamo_Mendelev_Han_Fe_2__MO_769582363439_000
EAM_Dynamo_Mendelev_Han_Fe_5	EAM_Dynamo_Mendelev_Han_Fe_5__MO_942420706858_000
EAM_Dynamo_Mendelev_Han_VFe	EAM_Dynamo_Mendelev_Han_VFe__MO_249706810527_000
EAM_Dynamo_Mendelev_King_Cu	EAM_Dynamo_Mendelev_King_Cu__MO_748636486270_000
EAM_Dynamo_Mendelev_Kramer_Al	EAM_Dynamo_Mendelev_Kramer_Al__MO_106969701023_000
EAM_Dynamo_Mendelev_Kramer_Cu	EAM_Dynamo_Mendelev_Kramer_Cu__MO_945691923444_000
EAM_Dynamo_Mendelev_Kramer_CuZr	EAM_Dynamo_Mendelev_Kramer_CuZr__MO_600021860456_000
EAM_Dynamo_Mendelev_Ni	EAM_Dynamo_Mendelev_Ni__MO_832600236922_000
EAM_Dynamo_Mendelev_NiZr	EAM_Dynamo_Mendelev_NiZr__MO_149104665840_000
EAM_Dynamo_Mendelev_Sordelet_CuZr	EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_000
EAM_Dynamo_Mendelev_Srolovitz_AlFe	EAM_Dynamo_Mendelev_Srolovitz_AlFe__MO_577453891941_000
EAM_Dynamo_Mishin_Farkas_Al	EAM_Dynamo_Mishin_Farkas_Al__MO_651801486679_000
EAM_Dynamo_Mishin_Farkas_Ni	EAM_Dynamo_Mishin_Farkas_Ni__MO_400591584784_000
EAM_Dynamo_Mishin_Mehl_Cu	EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_000
EAM_Dynamo_Mishin_Mehl_NiAl	EAM_Dynamo_Mishin_Mehl_NiAl__MO_109933561507_000
EAM_Dynamo_Mishin_NiAl	EAM_Dynamo_Mishin_NiAl__MO_101214310689_000
EAM_Dynamo_Passianot_Vailhe_Voter_CoAl	EAM_Dynamo_Passianot_Vailhe_Voter_CoAl__MO_284963179498_000
EAM_Dynamo_PurjaPun_Mishin_Co	EAM_Dynamo_PurjaPun_Mishin_Co__MO_885079680379_000
EAM_Dynamo_PurjaPun_Mishin_NiAl	EAM_Dynamo_PurjaPun_Mishin_NiAl__MO_751354403791_000
EAM_Dynamo_Smirnova_U	EAM_Dynamo_Smirnova_U__MO_126659884885_000
EAM_Dynamo_Smirnova_UMoXe	EAM_Dynamo_Smirnova_UMoXe__MO_679329885632_000
EAM_Dynamo_Sturgeon_Laird_Al	EAM_Dynamo_Sturgeon_Laird_Al__MO_120808805541_000
EAM_Dynamo_Sun_Mendelev_Mg	EAM_Dynamo_Sun_Mendelev_Mg__MO_848345414202_000
EAM_Dynamo_Williams_Mishin_Ag	EAM_Dynamo_Williams_Mishin_Ag__MO_131620013077_000
EAM_Dynamo_Williams_Mishin_CuAg	EAM_Dynamo_Williams_Mishin_CuAg__MO_128703483589_000
EAM_Dynamo_Winey_Kubota_Al	EAM_Dynamo_Winey_Kubota_Al__MO_149316865608_000
EAM_Dynamo_Wu_Trinkle_CuAg	EAM_Dynamo_Wu_Trinkle_CuAg__MO_270337113239_000
EAM_Dynamo_Zhou_Johnson_Ag	EAM_Dynamo_Zhou_Johnson_Ag__MO_947112899505_000
EAM_Dynamo_Zhou_Johnson_Al	EAM_Dynamo_Zhou_Johnson_Al__MO_131650261510_000
EAM_Dynamo_Zhou_Johnson_Au	EAM_Dynamo_Zhou_Johnson_Au__MO_468407568810_000
EAM_Dynamo_Zhou_Johnson_Co	EAM_Dynamo_Zhou_Johnson_Co__MO_924630542818_000
EAM_Dynamo_Zhou_Johnson_Cu	EAM_Dynamo_Zhou_Johnson_Cu__MO_127245782811_000
EAM_Dynamo_Zhou_Johnson_Fe	EAM_Dynamo_Zhou_Johnson_Fe__MO_650279905230_000
EAM_Dynamo_Zhou_Johnson_Mg	EAM_Dynamo_Zhou_Johnson_Mg__MO_137404467969_000
EAM_Dynamo_Zhou_Johnson_Mo	EAM_Dynamo_Zhou_Johnson_Mo__MO_271256517527_000
EAM_Dynamo_Zhou_Johnson_Ni	EAM_Dynamo_Zhou_Johnson_Ni__MO_110256178378_000
EAM_Dynamo_Zhou_Johnson_Pb	EAM_Dynamo_Zhou_Johnson_Pb__MO_116920074573_000
EAM_Dynamo_Zhou_Johnson_Pt	EAM_Dynamo_Zhou_Johnson_Pt__MO_102190350384_000
EAM_Dynamo_Zhou_Johnson_Ta	EAM_Dynamo_Zhou_Johnson_Ta__MO_130046220009_000
EAM_Dynamo_Zhou_Johnson_Ti	EAM_Dynamo_Zhou_Johnson_Ti__MO_723456820410_000
EAM_Dynamo_Zhou_Johnson_W	EAM_Dynamo_Zhou_Johnson_W__MO_524392058194_000
EAM_Dynamo_Zhou_Johnson_Zr	EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000
EAM_Dynamo_Zope_Mishin_Al	EAM_Dynamo_Zope_Mishin_Al__MO_664470114311_000
EAM_Dynamo_Zope_Mishin_TiAl	EAM_Dynamo_Zope_Mishin_TiAl__MO_117656786760_000

IMD_EAM__MD_113599595631_000

Title	Extended KIM ID
IMD_AlMnPd	IMD_AlMnPd__MO_878712978062_000
IMD_AlNiCo_A	IMD_AlNiCo_A__MO_122703700223_000
IMD_AlNiCo_B	IMD_AlNiCo_B__MO_128037485276_000
IMD_CaCd	IMD_CaCd__MO_145183423516_000
IMD_MgZn	IMD_MgZn__MO_710767216198_000

TB_FinnisSinclair_F__MD_110268284761_000

Title	Extended KIM ID
TB_FinnisSinclair_F_Cr	TB_FinnisSinclair_F_Cr__MO_978292918201_000
TB_FinnisSinclair_F_Fe	TB_FinnisSinclair_F_Fe__MO_128043931343_000
TB_FinnisSinclair_F_Mo	TB_FinnisSinclair_F_Mo__MO_137948437492_000
TB_FinnisSinclair_F_Nb	TB_FinnisSinclair_F_Nb__MO_264460139880_000
TB_FinnisSinclair_F_Ta	TB_FinnisSinclair_F_Ta__MO_161779068577_000
TB_FinnisSinclair_F_V	TB_FinnisSinclair_F_V__MO_792314740411_000
TB_FinnisSinclair_F_W	TB_FinnisSinclair_F_W__MO_115134210350_000

TB_Khakshouri_F__MD_334656137685_000

Title	Extended KIM ID
TB_Khakshouri_F_Cr	TB_Khakshouri_F_Cr__MO_102638147660_000
TB_Khakshouri_F_Fe	TB_Khakshouri_F_Fe__MO_114358763319_000
TB_Khakshouri_F_Mo	TB_Khakshouri_F_Mo__MO_114301908431_000
TB_Khakshouri_F_Nb	TB_Khakshouri_F_Nb__MO_560494786128_000
TB_Khakshouri_F_Ta	TB_Khakshouri_F_Ta__MO_133010535242_000
TB_Khakshouri_F_V	TB_Khakshouri_F_V__MO_571745055869_000
TB_Khakshouri_F_W	TB_Khakshouri_F_W__MO_109937641569_000

asap_emt_driver__MD_128315414717_000

Title	Extended KIM ID
asap_emt	asap_emt__MO_118428466217_000

ex_model_driver_P_LJ__MD_498634107543_000

Title	Extended KIM ID
ex_model_Ar_P_LJ	ex_model_Ar_P_LJ__MO_129904326346_000
ex_model_Ne_P_LJ	ex_model_Ne_P_LJ__MO_135498364023_000

ex_model_driver_P_Morse__MD_552566534109_000

Title	Extended KIM ID
ex_model_Ar_P_Morse	ex_model_Ar_P_Morse__MO_831902330215_000
ex_model_Ne_P_Morse	ex_model_Ne_P_Morse__MO_169434419764_000

kcc_meam_driver__MD_111291751625_000

Title	Extended KIM ID
kcc_meam_Fe_to_Ga	kcc_meam_Fe_to_Ga__MO_145522277939_000
kcc_meam_GaInN	kcc_meam_GaInN__MO_117938381510_000
kcc_meam_LiSi	kcc_meam_LiSi__MO_596436139350_000

kcc_model_driver_T_SW__MD_335816936951_000

Title	Extended KIM ID
kcc_model_Si_T_SW	kcc_model_Si_T_SW__MO_405512056662_000

model_driver_PF_cubic_splines__MD_620624592962_000

Title	Extended KIM ID
model_Fe_PF_DudarevDerlet	model_Fe_PF_DudarevDerlet__MO_135034229282_000
model_Fe_PF_mendelev	model_Fe_PF_mendelev__MO_856295952425_000
model_Mo_PF_cubicsplines	model_Mo_PF_cubicsplines__MO_424746498193_000
model_Nb_PF_cubicsplines	model_Nb_PF_cubicsplines__MO_218026715338_000
model_Ta_PF_cubicsplines	model_Ta_PF_cubicsplines__MO_261274272789_000
model_V_PF_cubicsplines	model_V_PF_cubicsplines__MO_683890323730_000
model_W_PF_cubicsplines	model_W_PF_cubicsplines__MO_195478838873_000

model_driver_PF_quintic_splines__MD_543355979582_000

Title	Extended KIM ID
model_Fe_PF_chiesa_quinticsplines	model_Fe_PF_chiesa_quinticsplines__MO_140444321607_000

model_driver_Si_BOP_EDIP_C__MD_506186535567_000

Title	Extended KIM ID
model_Si_BOP_EDIP_C	model_Si_BOP_EDIP_C__MO_958932894036_000

No Driver

Title	Extended KIM ID
ex_model_Al_PF_ErcolessiAdams	ex_model_Al_PF_ErcolessiAdams__MO_324507536345_000
ex_model_Ar_P_MLJ_C	ex_model_Ar_P_MLJ_C__MO_412414474378_000
ex_model_Ar_P_MLJ_CLUSTER_C	ex_model_Ar_P_MLJ_CLUSTER_C__MO_109568282781_000
ex_model_Ar_P_MLJ_CLUSTER_F90	ex_model_Ar_P_MLJ_CLUSTER_F90__MO_102380223850_000
ex_model_Ar_P_MLJ_F90	ex_model_Ar_P_MLJ_F90__MO_597866518552_000
ex_model_Ar_P_MLJ_MI_OPBC_H_F	ex_model_Ar_P_MLJ_MI_OPBC_H_F__MO_102974499161_000
ex_model_Ar_P_MLJ_NEIGH_PURE_H_F	ex_model_Ar_P_MLJ_NEIGH_PURE_H_F__MO_142368339264_000
ex_model_Ar_P_MLJ_NEIGH_RVEC_F	ex_model_Ar_P_MLJ_NEIGH_RVEC_F__MO_127655546155_000
ex_model_ArNe_P_MLJ_NEIGH_RVEC_F	ex_model_ArNe_P_MLJ_NEIGH_RVEC_F__MO_127340753366_000
ex_model_Cu_PF_Johnson	ex_model_Cu_PF_Johnson__MO_887933271505_000
ex_model_Ne_P_fastLJ	ex_model_Ne_P_fastLJ__MO_891816029319_000
ex_model_Ne_P_LJ_NEIGH_PURE_H	ex_model_Ne_P_LJ_NEIGH_PURE_H__MO_103464740545_000
ex_model_Ne_P_MLJ_NEIGH_RVEC_H	ex_model_Ne_P_MLJ_NEIGH_RVEC_H__MO_117820694701_000
iron_pair_potential	iron_pair_potential__MO_857282754307_000
kcc_model_exp6	kcc_model_exp6__MO_946046425752_000
model_ArCHHeXe_BOP_AIREBO	model_ArCHHeXe_BOP_AIREBO__MO_154399806462_000
model_Cu_PF_Johnson	model_Cu_PF_Johnson__MO_129229327064_000
model_He_P_Abln	model_He_P_Abln__MO_126942667206_000
model_Si_3B_Stillinger_Weber	model_Si_3B_Stillinger_Weber__MO_588169812045_000
model_YSZ_PF_Dipole	model_YSZ_PF_Dipole__MO_394669891912_000

1 »

Model model_Si_3B_Stillinger_Weber__MO_588169812045_000

Title	model_Si_3B_Stillinger_Weber
Short KIM ID	MO_588169812045_000
Extended KIM ID	model_Si_3B_Stillinger_Weber__MO_588169812045_000
Species	Si
Description	
Details	
Disclaimer	
Driver	

Tests

(paired to Model through Test Result)

Test	Test Result
Cluster_100_Si__TE_429523702910_000	view
Cluster_101_Si__TE_931357417688_000	view
Cluster_102_Si__TE_899934259195_000	view
Cluster_103_Si__TE_208571514677_000	view
Cluster_104_Si__TE_432205369431_000	view
Cluster_105_Si__TE_980317120430_000	view
Cluster_106_Si__TE_994447413828_000	view
Cluster_107_Si__TE_488400057650_000	view
Cluster_108_Si__TE_287178825254_000	view
Cluster_109_Si__TE_998136504085_000	view
Cluster_10_Si__TE_528551716137_000	view
Cluster_110_Si__TE_853588156798_000	view
Cluster_111_Si__TE_031086338232_000	view
Cluster_112_Si__TE_930486899301_000	view
Cluster_113_Si__TE_531412975643_000	view
Cluster_114_Si__TE_871942700757_000	view
Cluster_115_Si__TE_054330094742_000	view
Cluster_116_Si__TE_976541780854_000	view
Cluster_117_Si__TE_479981760251_000	view
Cluster_118_Si__TE_891613298510_000	view
Cluster_119_Si__TE_096187425822_000	view
Cluster_11_Si__TE_035980411356_000	view
Cluster_120_Si__TE_234587886945_000	view
Cluster_121_Si__TE_632487195837_000	view
Cluster_122_Si__TE_538728071627_000	view
Cluster_123_Si__TE_306925050125_000	view
Cluster_124_Si__TE_844531965834_000	view
Cluster_125_Si__TE_533257083749_000	view
Cluster_126_Si__TE_756219814882_000	view
Cluster_127_Si__TE_615549475706_000	view
Cluster_128_Si__TE_734283857388_000	view
Cluster_129_Si__TE_038600500690_000	view
Cluster_12_Si__TE_455598598557_000	view
Cluster_130_Si__TE_597583397103_000	view
Cluster_131_Si__TE_163807559834_000	view
Cluster_132_Si__TE_969957918845_000	view
Cluster_133_Si__TE_497517655834_000	view
Cluster_134_Si__TE_372379074977_000	view
Cluster_135_Si__TE_402163287811_000	view
Cluster_136_Si__TE_477834775800_000	view
Cluster_137_Si__TE_366826488341_000	view
Cluster_138_Si__TE_890563345462_000	view
Cluster_139_Si__TE_765013601520_000	view
Cluster_13_Si__TE_456277203492_000	view
Cluster_140_Si__TE_364962991962_000	view
Cluster_141_Si__TE_744151501796_000	view
Cluster_142_Si__TE_796099939753_000	view
Cluster_143_Si__TE_295449890799_000	view
Cluster_144_Si__TE_275564477441_000	view
Cluster_145_Si__TE_668042640512_000	view
Cluster_146_Si__TE_349779986007_000	view
Cluster_147_Si__TE_252106257831_000	view
Cluster_148_Si__TE_148024400299_000	view
Cluster_149_Si__TE_241393284053_000	view
Cluster_14_Si__TE_703475516150_000	view
Cluster_150_Si__TE_348293683653_000	view
Cluster_151_Si__TE_382612287244_000	view
Cluster_152_Si__TE_873880479890_000	view
Cluster_153_Si__TE_887021755280_000	view
Cluster_154_Si__TE_689537337370_000	view
Cluster_155_Si__TE_718412445260_000	view
Cluster_156_Si__TE_420278838565_000	view
Cluster_157_Si__TE_445757151788_000	view
Cluster_158_Si__TE_333961920502_000	view
Cluster_159_Si__TE_154562695955_000	view
Cluster_15_Si__TE_063996320154_000	view
Cluster_160_Si__TE_484357652945_000	view
Cluster_161_Si__TE_931545318071_000	view
Cluster_162_Si__TE_318370255789_000	view
Cluster_163_Si__TE_454315571325_000	view
Cluster_164_Si__TE_429062973441_000	view
Cluster_165_Si__TE_690749330767_000	view
Cluster_166_Si__TE_856478859137_000	view
Cluster_167_Si__TE_906897749707_000	view
Cluster_168_Si__TE_057575819109_000	view
Cluster_169_Si__TE_747042204134_000	view
Cluster_16_Si__TE_210985104651_000	view
Cluster_170_Si__TE_671911350763_000	view
Cluster_171_Si__TE_422538811071_000	view
Cluster_172_Si__TE_491193705466_000	view
Cluster_173_Si__TE_468011290052_000	view
Cluster_174_Si__TE_717988702336_000	view
Cluster_175_Si__TE_766758182907_000	view
Cluster_176_Si__TE_136053930099_000	view
Cluster_177_Si__TE_067768687879_000	view
Cluster_178_Si__TE_018864440740_000	view
Cluster_179_Si__TE_284078330399_000	view
Cluster_17_Si__TE_753646674916_000	view
Cluster_180_Si__TE_309161971932_000	view
Cluster_181_Si__TE_367158124393_000	view
Cluster_182_Si__TE_666690617643_000	view
Cluster_183_Si__TE_183042451358_000	view
Cluster_184_Si__TE_254179879675_000	view
Cluster_185_Si__TE_356227955015_000	view
Cluster_186_Si__TE_901454897084_000	view
Cluster_187_Si__TE_674458718240_000	view
Cluster_188_Si__TE_801985106803_000	view
Cluster_189_Si__TE_235416817122_000	view
Cluster_18_Si__TE_210566963632_000	view
Cluster_190_Si__TE_829021414195_000	view
Cluster_191_Si__TE_286342759284_000	view
Cluster_192_Si__TE_166962134729_000	view
Cluster_193_Si__TE_147391669986_000	view
Cluster_194_Si__TE_740658330609_000	view
Cluster_195_Si__TE_596025108636_000	view
Cluster_196_Si__TE_838141000753_000	view
Cluster_197_Si__TE_597137189282_000	view
Cluster_198_Si__TE_502922857879_000	view
Cluster_199_Si__TE_895716819862_000	view
Cluster_19_Si__TE_710848114317_000	view
Cluster_1_Si__TE_587715205790_000	view
Cluster_200_Si__TE_344179392952_000	view
Cluster_201_Si__TE_174834208178_000	view
Cluster_202_Si__TE_318255630935_000	view
Cluster_203_Si__TE_835373098884_000	view
Cluster_204_Si__TE_642845498230_000	view
Cluster_205_Si__TE_036244332807_000	view
Cluster_206_Si__TE_602131281327_000	view
Cluster_207_Si__TE_778899428796_000	view
Cluster_208_Si__TE_104013020686_000	view
Cluster_209_Si__TE_620995722068_000	view
Cluster_20_Si__TE_003643308767_000	view
Cluster_210_Si__TE_062977758731_000	view
Cluster_211_Si__TE_413174992619_000	view
Cluster_212_Si__TE_988153846927_000	view
Cluster_213_Si__TE_729668376840_000	view
Cluster_214_Si__TE_596217443977_000	view
Cluster_215_Si__TE_242333726138_000	view
Cluster_216_Si__TE_085896331391_000	view
Cluster_217_Si__TE_497672340598_000	view
Cluster_218_Si__TE_916792444379_000	view
Cluster_219_Si__TE_887881438194_000	view
Cluster_21_Si__TE_659903041393_000	view
Cluster_220_Si__TE_733089158186_000	view
Cluster_221_Si__TE_745813858576_000	view
Cluster_222_Si__TE_174224197479_000	view
Cluster_223_Si__TE_900051292915_000	view
Cluster_224_Si__TE_893205528562_000	view
Cluster_225_Si__TE_914882528089_000	view
Cluster_226_Si__TE_496076401087_000	view
Cluster_227_Si__TE_731346528851_000	view
Cluster_228_Si__TE_512019717372_000	view
Cluster_229_Si__TE_998999258967_000	view
Cluster_22_Si__TE_262831495731_000	view
Cluster_230_Si__TE_627063348715_000	view
Cluster_231_Si__TE_856199110324_000	view
Cluster_232_Si__TE_173833466681_000	view
Cluster_233_Si__TE_945318979650_000	view
Cluster_234_Si__TE_691572208744_000	view
Cluster_235_Si__TE_816678965378_000	view
Cluster_236_Si__TE_981563312457_000	view
Cluster_237_Si__TE_293703490073_000	view
Cluster_238_Si__TE_595578393709_000	view
Cluster_239_Si__TE_085576332679_000	view
Cluster_23_Si__TE_454667266203_000	view
Cluster_240_Si__TE_914699212141_000	view
Cluster_241_Si__TE_658556152441_000	view
Cluster_242_Si__TE_498751325298_000	view
Cluster_243_Si__TE_902853058604_000	view
Cluster_244_Si__TE_388224528817_000	view
Cluster_245_Si__TE_094968768812_000	view
Cluster_246_Si__TE_145186784279_000	view
Cluster_247_Si__TE_474120860208_000	view
Cluster_248_Si__TE_592641109876_000	view
Cluster_249_Si__TE_061979228659_000	view
Cluster_24_Si__TE_670233848350_000	view
Cluster_250_Si__TE_362002298404_000	view
Cluster_251_Si__TE_325730267597_000	view
Cluster_252_Si__TE_807793087235_000	view
Cluster_253_Si__TE_536226495883_000	view
Cluster_254_Si__TE_225781560049_000	view
Cluster_255_Si__TE_700998615333_000	view
Cluster_256_Si__TE_451109023508_000	view
Cluster_257_Si__TE_721857961602_000	view
Cluster_258_Si__TE_432345143720_000	view
Cluster_259_Si__TE_963128740881_000	view
Cluster_25_Si__TE_521947206240_000	view
Cluster_260_Si__TE_720857220105_000	view
Cluster_261_Si__TE_059408491970_000	view
Cluster_262_Si__TE_819327851206_000	view
Cluster_263_Si__TE_894690687252_000	view
Cluster_264_Si__TE_004727471156_000	view
Cluster_265_Si__TE_510900059486_000	view
Cluster_266_Si__TE_711369652165_000	view
Cluster_267_Si__TE_986290783614_000	view
Cluster_268_Si__TE_804603549560_000	view
Cluster_269_Si__TE_306948045411_000	view
Cluster_26_Si__TE_907212854318_000	view
Cluster_270_Si__TE_071867115829_000	view
Cluster_271_Si__TE_719302761702_000	view
Cluster_272_Si__TE_965504197852_000	view
Cluster_273_Si__TE_570618441127_000	view
Cluster_274_Si__TE_622155819842_000	view
Cluster_275_Si__TE_353728726670_000	view
Cluster_276_Si__TE_665587210405_000	view
Cluster_277_Si__TE_767342604587_000	view
Cluster_278_Si__TE_827849586878_000	view
Cluster_279_Si__TE_258228319817_000	view
Cluster_27_Si__TE_379384370231_000	view
Cluster_280_Si__TE_829321833247_000	view
Cluster_281_Si__TE_189851884818_000	view
Cluster_282_Si__TE_583958587414_000	view
Cluster_283_Si__TE_637114920018_000	view
Cluster_284_Si__TE_726078380702_000	view
Cluster_285_Si__TE_809740147463_000	view
Cluster_286_Si__TE_338113534887_000	view
Cluster_287_Si__TE_177187404211_000	view
Cluster_288_Si__TE_531598108601_000	view
Cluster_289_Si__TE_770458678607_000	view
Cluster_28_Si__TE_190150687559_000	view
Cluster_290_Si__TE_140316144628_000	view
Cluster_291_Si__TE_252455328708_000	view
Cluster_292_Si__TE_829867171043_000	view
Cluster_293_Si__TE_959643995835_000	view
Cluster_294_Si__TE_147146015496_000	view
Cluster_295_Si__TE_834594642199_000	view
Cluster_296_Si__TE_470544055322_000	view
Cluster_297_Si__TE_858515667662_000	view
Cluster_298_Si__TE_820885425814_000	view
Cluster_299_Si__TE_275147604418_000	view
Cluster_29_Si__TE_648378160617_000	view
Cluster_2_Si__TE_888062595336_000	view
Cluster_300_Si__TE_165463712608_000	view
Cluster_301_Si__TE_892752541643_000	view
Cluster_302_Si__TE_994450366120_000	view
Cluster_303_Si__TE_130967909996_000	view
Cluster_304_Si__TE_463370982772_000	view
Cluster_305_Si__TE_616606185964_000	view
Cluster_306_Si__TE_484696636667_000	view
Cluster_307_Si__TE_128958192713_000	view
Cluster_308_Si__TE_383948790087_000	view
Cluster_309_Si__TE_312546223547_000	view
Cluster_30_Si__TE_171163969287_000	view
Cluster_310_Si__TE_387186512530_000	view
Cluster_311_Si__TE_213270622870_000	view
Cluster_312_Si__TE_502398108365_000	view
Cluster_313_Si__TE_971145099945_000	view
LatticeConstantCubicEnergy_Si_bcc__TE_534114247034_000	view
LatticeConstantCubicEnergy_Si_diamond__TE_849680434885_000	view
LatticeConstantCubicEnergy_Si_fcc__TE_828776015817_000	view
LatticeConstantCubicEnergy_Si_sc__TE_445489171948_000	view

Visualizers

- Atomic Configurations
- Lattice Constant
- Cohesive Energy
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- Phonon Dispersion Relation Curve

Files

Files
Makefile
README
kimspec.ini
model_Si_3B_Stillinger_Weber.c
model_Si_3B_Stillinger_Weber__MO_588169812045_000.kim

Model EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000

Title	EAM_Dynamo_Ercolessi_Adams_Al
Short KIM ID	MO_123629422045_000
Extended KIM ID	EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000
Species	Al
Description	
Details	
Disclaimer	
Driver	EAM_Dynamo__MD_120291908751_000

Tests

(paired to Model through Test Result)

Test	Test Result
LatticeConstantCubicEnergy_Al_bcc__TE_201065028814_000	view
LatticeConstantCubicEnergy_Al_diamond__TE_586085652256_000	view
LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000	view
LatticeConstantCubicEnergy_Al_sc__TE_272202056996_000	view
PhononDispersionCurve_Al_fcc__TE_363050395011_000	view
SurfaceTest_Al_fcc__TE_761372278666_000	view

Visualizers

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Files

Files
Al_EA.eam.alloy
Makefile
kimspec.ini

Model Driver EAM_Dynamo__MD_120291908751_000

Title	EAM_Dynamo
Short KIM ID	MD_120291908751_000
Extended KIM ID	EAM_Dynamo__MD_120291908751_000
Species	
Description	
Details	
Disclaimer	

Models using this Model Driver

EAM_Dynamo_Ackland_Bacon_Fe__MO_142799717516_000
EAM_Dynamo_Ackland_Mendelev_FeP__MO_884343146310_000
EAM_Dynamo_Ackland_Ti__MO_748534961139_000
EAM_Dynamo_Ackland_Tichy_Ag__MO_212700056563_000
EAM_Dynamo_Ackland_Tichy_Au__MO_104891429740_000
EAM_Dynamo_Ackland_Tichy_Cu__MO_179025990738_000
EAM_Dynamo_Ackland_Tichy_Ni__MO_977363131043_000
EAM_Dynamo_Ackland_W__MO_141627196590_000
EAM_Dynamo_Adams_Foiles_Ag_u4__MO_366710161005_000
EAM_Dynamo_Adams_Foiles_Au_u4__MO_542075092223_000
EAM_Dynamo_Adams_Foiles_Cu_u4__MO_783346091107_000
EAM_Dynamo_Adams_Foiles_Ni_u4__MO_130989848973_000
EAM_Dynamo_Adams_Foiles_Pt_u4__MO_117515733772_000
EAM_Dynamo_Angelo_Moody_NiAlH__MO_418978237058_000
EAM_Dynamo_Bonny_Pasianot_FeCuNi__MO_469343973171_000
EAM_Dynamo_Bonny_Pasianot_FeNi__MO_267721408934_000
EAM_Dynamo_Cai_Ye_AlCu__MO_942551040047_000
EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000
EAM_Dynamo_Fellinger_Park_Nb__MO_102133002179_000
EAM_Dynamo_Foiles_CuNi__MO_869958188303_000
EAM_Dynamo_Foiles_Cu_u3__MO_468316472729_000
EAM_Dynamo_Fortini_Mendelev_Ru__MO_114077951467_000
EAM_Dynamo_Grochola_Russo_Au__MO_852752408985_000
EAM_Dynamo_Hepburn_Ackland_FeC__MO_143977152728_000
EAM_Dynamo_Hoyt_Garvin_PbCu__MO_119135752160_000
EAM_Dynamo_Landa_Wynblatt_AlPb__MO_699137396381_000
EAM_Dynamo_Li_Siegel_Ta__MO_103054252769_000
EAM_Dynamo_Liu_Adams_MgAl__MO_544273640230_000
EAM_Dynamo_Liu_Ercolessi_Al__MO_194915988663_000
EAM_Dynamo_Liu_Liu_AlCu__MO_128706169020_000
EAM_Dynamo_Liu_Liu_Liu_AlFe__MO_503784222035_000
EAM_Dynamo_Liu_Ohotnicky_MgAl__MO_135676685253_000
EAM_Dynamo_Mendelev_Asta_AlMg__MO_658278549784_000
EAM_Dynamo_Mendelev_Han_Fe_2__MO_769582363439_000
EAM_Dynamo_Mendelev_Han_Fe_5__MO_942420706858_000
EAM_Dynamo_Mendelev_Han_VFe__MO_249706810527_000
EAM_Dynamo_Mendelev_King_Cu__MO_748636486270_000
EAM_Dynamo_Mendelev_Kramer_Al__MO_106969701023_000
EAM_Dynamo_Mendelev_Kramer_CuZr__MO_600021860456_000
EAM_Dynamo_Mendelev_Kramer_Cu__MO_945691923444_000
EAM_Dynamo_Mendelev_NiZr__MO_149104665840_000
EAM_Dynamo_Mendelev_Ni__MO_832600236922_000
EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_000
EAM_Dynamo_Mendelev_Srolovitz_AlFe__MO_577453891941_000
EAM_Dynamo_Mishin_Farkas_Al__MO_651801486679_000
EAM_Dynamo_Mishin_Farkas_Ni__MO_400591584784_000
EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_000
EAM_Dynamo_Mishin_Mehl_NiAl__MO_109933561507_000
EAM_Dynamo_Mishin_NiAl__MO_101214310689_000
EAM_Dynamo_Passianot_Vailhe_Voter_CoAl__MO_284963179498_000
EAM_Dynamo_PurjaPun_Mishin_Co__MO_885079680379_000
EAM_Dynamo_PurjaPun_Mishin_NiAl__MO_751354403791_000
EAM_Dynamo_Smirnova_UMoXe__MO_679329885632_000
EAM_Dynamo_Smirnova_U__MO_126659884885_000
EAM_Dynamo_Sturgeon_Laird_Al__MO_120808805541_000
EAM_Dynamo_Sun_Mendelev_Mg__MO_848345414202_000
EAM_Dynamo_Williams_Mishin_Ag__MO_131620013077_000
EAM_Dynamo_Williams_Mishin_CuAg__MO_128703483589_000
EAM_Dynamo_Winey_Kubota_Al__MO_149316865608_000
EAM_Dynamo_Wu_Trinkle_CuAg__MO_270337113239_000
EAM_Dynamo_Zhou_Johnson_Ag__MO_947112899505_000
EAM_Dynamo_Zhou_Johnson_Al__MO_131650261510_000
EAM_Dynamo_Zhou_Johnson_Au__MO_468407568810_000
EAM_Dynamo_Zhou_Johnson_Co__MO_924630542818_000
EAM_Dynamo_Zhou_Johnson_Cu__MO_127245782811_000
EAM_Dynamo_Zhou_Johnson_Fe__MO_650279905230_000
EAM_Dynamo_Zhou_Johnson_Mg__MO_137404467969_000
EAM_Dynamo_Zhou_Johnson_Mo__MO_271256517527_000
EAM_Dynamo_Zhou_Johnson_Ni__MO_110256178378_000
EAM_Dynamo_Zhou_Johnson_Pb__MO_116920074573_000
EAM_Dynamo_Zhou_Johnson_Pt__MO_102190350384_000
EAM_Dynamo_Zhou_Johnson_Ta__MO_130046220009_000
EAM_Dynamo_Zhou_Johnson_Ti__MO_723456820410_000
EAM_Dynamo_Zhou_Johnson_W__MO_524392058194_000
EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000
EAM_Dynamo_Zope_Mishin_Al__MO_664470114311_000
EAM_Dynamo_Zope_Mishin_TiAl__MO_117656786760_000

Visualizers

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Files

Files

EAM_Dynamo.cpp
EAM_Dynamo.hpp
EAM_DynamoImplementation.cpp
EAM_DynamoImplementation.hpp
EAM_Dynamo__MD_120291908751_000.kim
LICENSE.CDDL
Makefile
kimspec.ini
legos/

KIM Items Properties Primitives

Test LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000

Title	LatticeConstantCubicEnergy_Al_fcc
Short KIM ID	TE_156715955670_000
Extended KIM ID	LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
Species	
Description	
Details	
Disclaimer	Computer generated
Driver	LatticeConstantCubicEnergy__TD_475411767977_000

Models

(paired to Test through Test Result)

Model	Test Result
EAM_Dynamo_Angelo_Moody_NiAlH__MO_418978237058_000	view
EAM_Dynamo_Cai_Ye_AlCu__MO_942551040047_000	view
EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000	view
EAM_Dynamo_Landa_Wynblatt_AlPb__MO_699137396381_000	view
EAM_Dynamo_Liu_Adams_MgAl__MO_544273640230_000	view
EAM_Dynamo_Liu_Ercolessi_Al__MO_194915988663_000	view
EAM_Dynamo_Liu_Liu_AlCu__MO_128706169020_000	view
EAM_Dynamo_Liu_Liu_AlFe__MO_503784222035_000	view
EAM_Dynamo_Liu_Ohotnicky_MgAl__MO_135676685253_000	view
EAM_Dynamo_Mendelev_Asta_AlMg__MO_658278549784_000	view
EAM_Dynamo_Mendelev_Kramer_Al__MO_106969701023_000	view
EAM_Dynamo_Mendelev_Srolovitz_AlFe__MO_577453891941_000	view
EAM_Dynamo_Mishin_Farkas_Al__MO_651801486679_000	view
EAM_Dynamo_Mishin_Mehl_NiAl__MO_109933561507_000	view
EAM_Dynamo_Mishin_NiAl__MO_101214310689_000	view
EAM_Dynamo_Passianot_Vailhe_Voter_CoAl__MO_284963179498_000	view
EAM_Dynamo_PurjaPun_Mishin_NiAl__MO_751354403791_000	view
EAM_Dynamo_Sturgeon_Laird_Al__MO_120808805541_000	view
EAM_Dynamo_Winey_Kubota_Al__MO_149316865608_000	view
EAM_Dynamo_Zhou_Johnson_Al__MO_131650261510_000	view
EAM_Dynamo_Zope_Mishin_Al__MO_664470114311_000	view
EAM_Dynamo_Zope_Mishin_TiAl__MO_117656786760_000	view
IMD_AlNiCo_A__MO_122703700223_000	view
IMD_AlNiCo_B__MO_128037485276_000	view
ex_model_Al_PF_ErcolessiAdams__MO_324507536345_000	view
kcc_meam_Fe_to_Ga__MO_145522277939_000	view

Visualizers

- Atomic Configurations
- Lattice Constant
- Cohesive Energy
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- Phonon Dispersion Relation Curve

Files

Files

- LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
- LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000.kim
- Makefile
- kimspec.ini
- output/
- pipeline.stdin
- pipeline.yaml

Test Drivers - Alphabetical

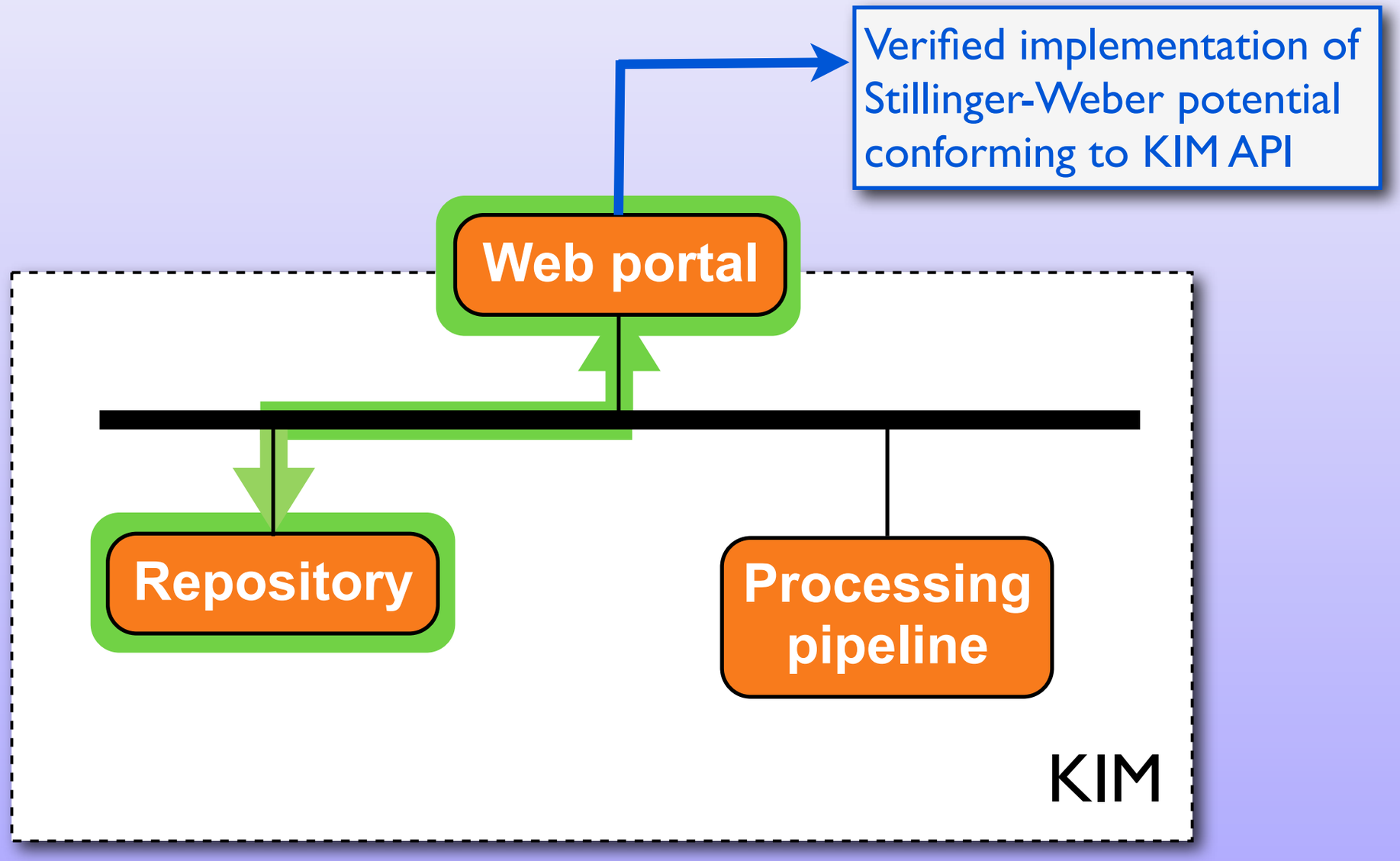
Title	Extended KIM ID
LatticeConstantCubicEnergy	LatticeConstantCubicEnergy__TD_475411767977_000
PhononDispersionCurve	PhononDispersionCurve__TD_530195868545_000
Potential energy and forces cluster test driver	Cluster__TD_000043093022_000
Potential energy and forces test driver for periodic triclinic boxes	TriclinicPBC__TD_892847239811_000
SurfaceTest	SurfaceTest__TD_955413365818_000

Reference Data - Alphabetical

Short KIM ID	Notes	Description
RD_001273404749_000	Submitted by Adam Ludvik, ludvi025@umn.edu	
RD_004043097245_000	Submitted by Adam Ludvik, ludvi025@umn.edu	
RD_004519572845_000	Submitted by Adam Ludvik, ludvi025@umn.edu	
RD_005343852019_000	Submitted by Adam Ludvik, ludvi025@umn.edu	
RD_006332579857_000	Submitted by Adam Ludvik, ludvi025@umn.edu	Comments about data: Internal Reference: Inorganic Crystal Structure Database; Temp reported as Room Temp; Pressure assumed to be standard;
RD_007612355138_000	Submitted by Adam Ludvik, ludvi025@umn.edu	Comments about data: excess Tl
RD_008797117656_000	Submitted by Adam Ludvik, ludvi025@umn.edu	
RD_010295044438_000	Submitted by Adam Ludvik, ludvi025@umn.edu	
RD_011497047262_000	Submitted by Adam Ludvik, ludvi025@umn.edu	Comments about data: Internal Reference: Inorganic Crystal Structure Database; Temp reported as Room Temp; Pressure assumed to be standard;
RD_012207314240_000	Submitted by Adam Ludvik, ludvi025@umn.edu	

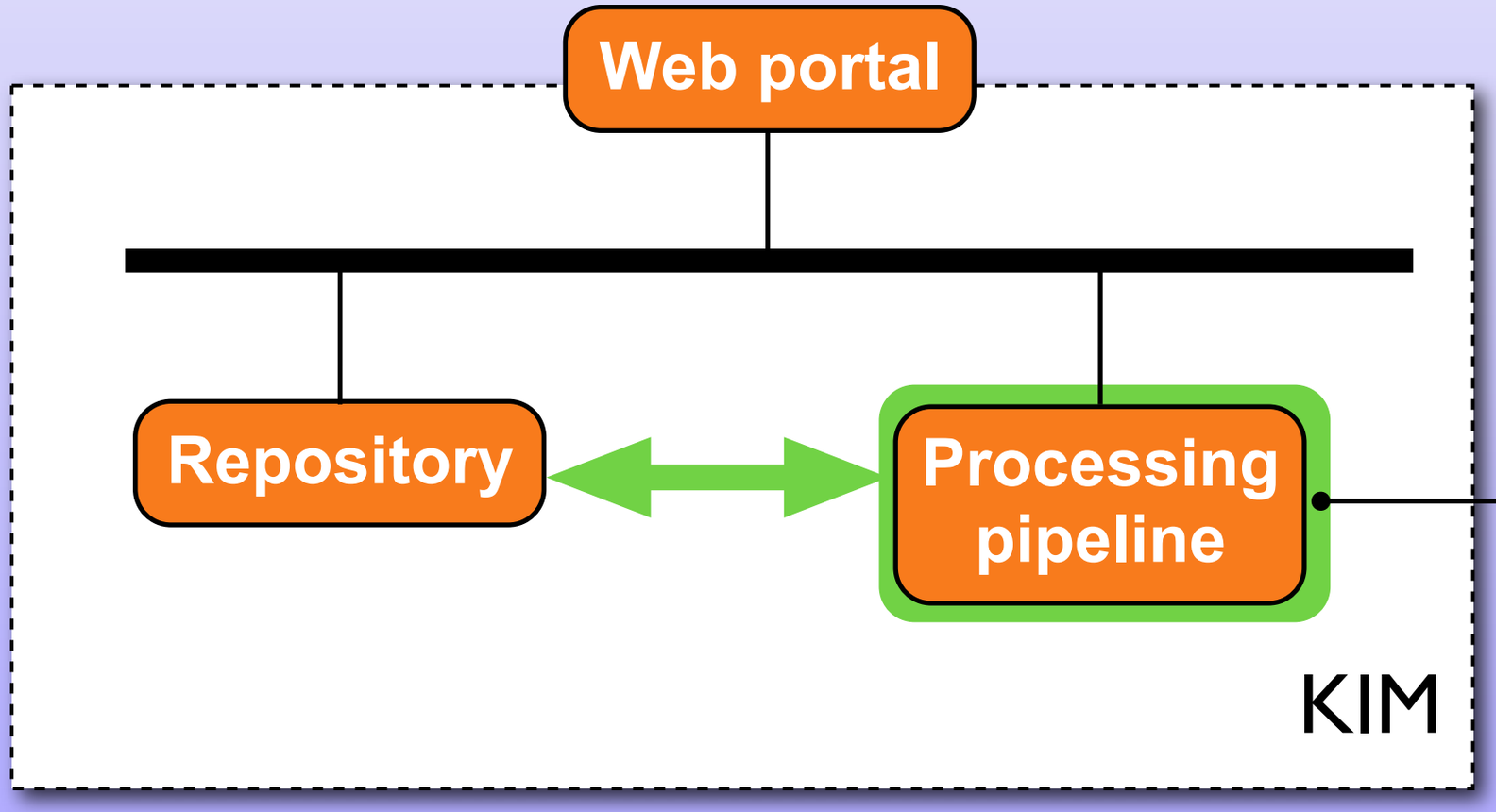
Interacting with KIM

Scenario I: Information query/retrieval

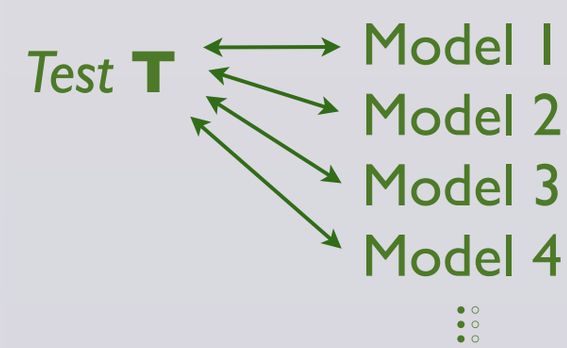


Interacting with KIM

Scenario II: Uploading new *Test*

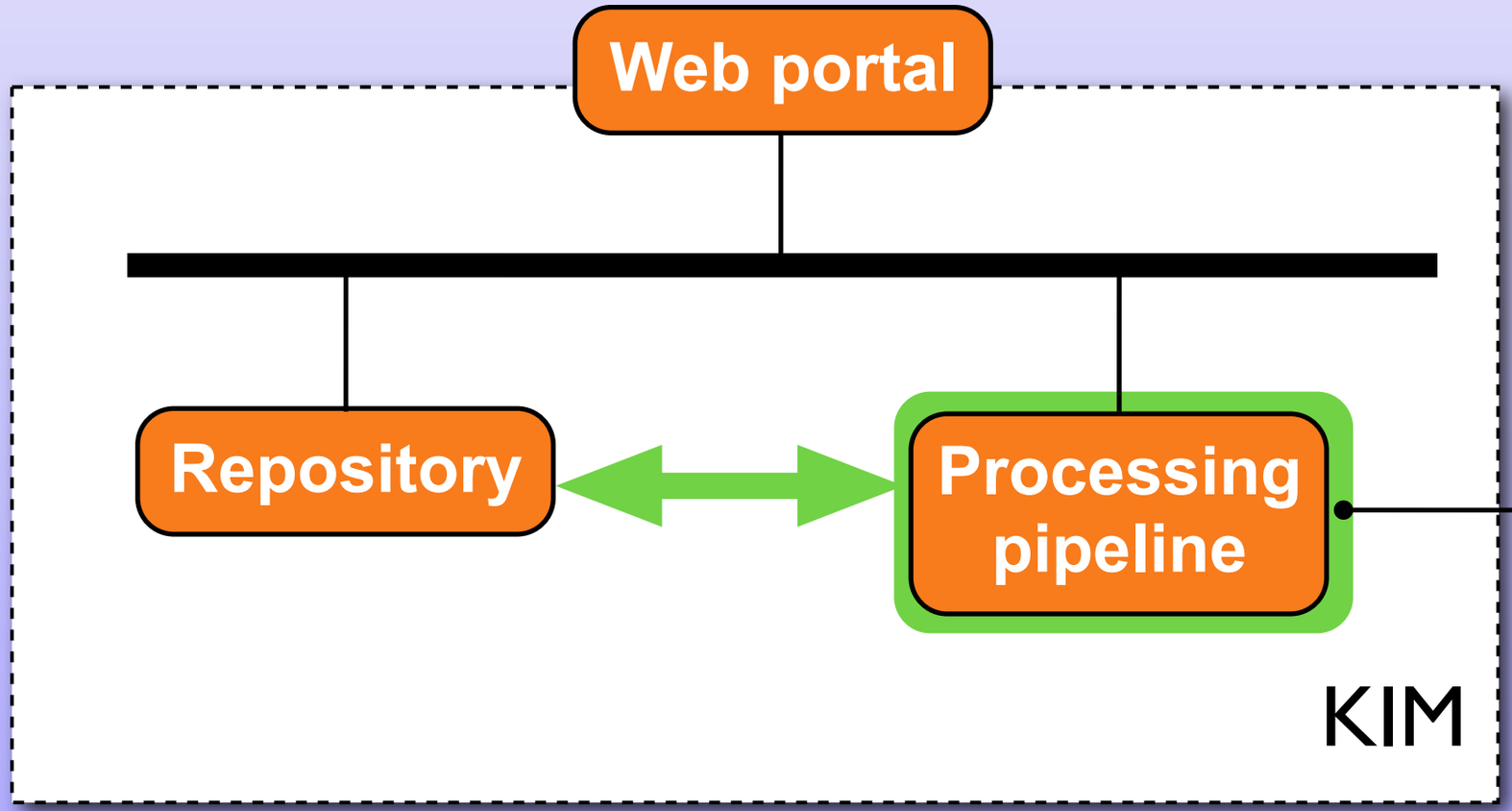


Couple *Test* **T** with all valid *Models* and store resulting *Predictions* in Repository.



Interacting with KIM

Scenario III: Uploading new *Model*



Couple *Model* **M** with all valid *Tests* and store resulting *Predictions* in Repository.

Model **M** ⟷ Test 1
Test 2
Test 3
Test 4
⋮

Web page demo of Pipeline, Test Results, and Visualization

cluster-potential-energy-and-forces

Key	Primitive
configuration-cluster	primitive/configuration-cluster
configuration-forces	primitive/configuration-forces
potential-energy	primitive/potential-energy

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:property/cluster-potential-energy-and-forces

cohesive-energy

Key	Primitive
crystal-structure	primitive/crystal-structure
energy	primitive/cohesive-energy
nvt	primitive/equilibrium-ensemble-nvt

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:property/cohesive-energy

equilibrium-crystal-structure

Key	Primitive
crystal-structure	primitive/crystal-structure
npt	primitive/equilibrium-ensemble-npt

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:property/equilibrium-crystal-structure

isothermal-bulk-modulus

Key	Primitive
crystal-structure	primitive/crystal-structure
isothermal-bulk-modulus	primitive/isothermal-bulk-modulus
nvt	primitive/equilibrium-ensemble-nvt

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:property/isothermal-bulk-modulus

phonon-density-of-states

Key	Primitive
crystal-structure	primitive/crystal-structure
dos	primitive/phonon-disperion-dos
nvt	primitive/equilibrium-ensemble-nvt

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:property/phonon-density-of-states

phonon-dispersion-plot

Key	Primitive
crystal-structure	primitive/crystal-structure
file	primitive/file
nvt	primitive/equilibrium-ensemble-nvt

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:property/phonon-dispersion-plot

phonon-dispersion-relation

Key	Primitive
crystal-structure	primitive/crystal-structure
kpoint	primitive/phonon-disperion-kpoint
nvt	primitive/equilibrium-ensemble-nvt
table-info	primitive/[reserved key]

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:property/phonon-dispersion-relation

cohesive-energy

Example

```
source-unit: eV/atom
source-value: 5.84
method-type: reference-data-experimental
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/cohesive-energy

configuration-cluster

Example

```
particle:
- contributing: true
  position-x:
    si-unit: m
    si-value: 3.025509e-10
    source-unit: angstrom
    source-value: 3.025509
  position-y:
    si-unit: m
    si-value: 3.351546e-10
    source-unit: angstrom
    source-value: 3.351546
  position-z:
    si-unit: m
    si-value: 8.965793e-11
    source-unit: angstrom
    source-value: 8.8965793
  species: Si
- contributing: true
  position-x:
    si-unit: m
    si-value: 3.226388e-10
    source-unit: angstrom
    source-value: 3.226388
  position-y:
    si-unit: m
    si-value: 7.458701e-11
    source-unit: angstrom
    source-value: 0.7458701
  position-z:
    si-unit: m
    si-value: 6.0328e-11
    source-unit: angstrom
    source-value: 0.60328
  species: Si
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/configuration-cluster

configuration-forces

Example

```
particle:
- contributing: true
  force-x:
    si-unit: m.kg.s-2
    si-value: -2.339358345660896e-10
    source-unit: eV/angstrom
    source-value: -0.1460112
  force-y:
    si-unit: m.kg.s-2
    si-value: -8.123436403077844e-10
    source-unit: eV/angstrom
    source-value: -0.5070248
  force-z:
    si-unit: m.kg.s-2
    si-value: -1.07095476815094e-09
    source-unit: eV/angstrom
    source-value: -0.6684371
  species: Si
- contributing: true
  force-x:
    si-unit: m.kg.s-2
    si-value: -2.982389012701 8e-10
    source-unit: eV/angstrom
    source-value: -0.186146
  force-y:
    si-unit: m.kg.s-2
    si-value: 1.140159905038 2e-09
    source-unit: eV/angstrom
    source-value: 0.711654
  force-z:
    si-unit: m.kg.s-2
    si-value: -5.663641857509 7e-10
    source-unit: eV/angstrom
    source-value: -0.353509
  species: Si
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/configuration-forces

crystal-structure

Example

```
a:
  source-unit: A
  source-value: 3.59
  method-type: reference-data-experimental
alpha:
  source-unit: degrees
  source-value: 90
  method-type: reference-data-experimental
b:
  source-unit: A
  source-value: 3.59
  method-type: reference-data-experimental
beta:
  source-unit: degrees
  source-value: 90
  method-type: reference-data-experimental
c:
  source-unit: A
  source-value: 5.65
  method-type: reference-data-experimental
gamma:
  source-unit: degrees
  source-value: 120
  method-type: reference-data-experimental
short-name:
- Dysprosium
- hcp
space-group: P6_3/mmc
wyckoff-site:
- code: 2c
  fract-x:
    source-unit: 1
    source-value: 0.3333333333
    method-type: reference-data-experimental
  fract-y:
    source-unit: 1
    source-value: 0.6666666666
    method-type: reference-data-experimental
  fract-z:
    source-unit: 1
    source-value: 0.25
    method-type: reference-data-experimental
  set-or-measured: measured
  species: Dy
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/crystal-structure

equilibrium-ensemble-npt

Example

```
temperature:
    source-unit: K
    source-value: 297
    method-type: reference-data-experimental
pressure:
    source-unit: atm
    source-value: 1
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/equilibrium-ensemble-npt

equilibrium-ensemble-nvt

Example

```
temperature:
    source-unit: K
    source-value: 297
    method-type: reference-data-experimental
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/equilibrium-ensemble-nvt

isothermal-bulk-modulus

Example

```
source-unit: 10^11 N/m^2
source-value: 0.384
method-type: reference-data-experimental
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/isothermal-bulk-modulus

kpoint

Example

```
response-frequency:
  si-unit: m2.kg.s-2
  si-value:
  - 3.3708653883333636e-29
  - 1.5090302036415 8e-22
  - 3.0117988513085e-22
  source-unit: meV
  source-value:
  - 2.1084216562553396e-07
  - 0.94186216181302 32
  - 1.8798161724941416
  table-info: phononcurve
wavelength:
  si-unit: m
  si-value:
  - 0.0
  - 6.1449116677 1e-12
  - 1.2288623335 4e-11
  - 1.8434735081e-11
  source-unit: angstrom
  source-value:
  - 0.0
  - 0.06144911667708593
  - 0.12288623335417185
  table-info: phononcurve
wavevector:
  ka:
    si-unit: m-1
    si-value:
    - 0.0
    - 0.0
    - 0.0
    source-unit: 1/angstrom
    source-value:
    - 0.0
    - 0.0
    - 0.0
  kb:
    si-unit: m-1
    si-value:
    - 200000000.0
    - 0.0
    - 200000000.0
    source-unit: 1/angstrom
    source-value:
    - 0.02
    - 0.0
    - 0.02
  kc:
    si-unit: m-1
    si-value:
    - 400000000.0
    - 0.0
    - 400000000.0
    source-unit: 1/angstrom
    source-value:
    - 0.04
    - 0.0
    - 0.04
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/kpoint

potential-energy

Example

```
si-unit: m2.kg.s-2
si-value: -1.1726567873547 4e-18
source-unit: eV
source-value: -7.3191448
```

KIM Namespace
tag:staff@noreply.openkim.org,2013-08-03:primitive/potential-energy

Pipeline logs

```
2013-08-06 00:42:06,485 - INFO - pipeline.template - attempting to process <open file '/home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running484b6d5c-fe29-11e2-84b6-34e1f30fc148__TE_107850120912_000/pipeline.stdin', mode 'r' at 0x3
5771e0> for ('EAM_Dynamo_Mendelev_NiZr__MO_149104665840_000','LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_00
0')
2013-08-06 00:42:06,495 - INFO - pipeline.compute - launching run...
2013-08-06 00:42:07,131 - INFO - pipeline.compute - Run completed in 0.6356160640716553 seconds
2013-08-06 00:42:07,669 - INFO - pipeline.compute - Copying the contents of /home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running484b6d5c-fe29-11e2-84b6-34e1f30fc148__TE_107850120912_000/output to /home/openkim/openkim-repository/
tr/484b6d5c-fe29-11e2-84b6-34e1f30fc148
2013-08-06 00:42:07,678 - INFO - pipeline.pipeline.worker-1 - Rsyncing results '484b6d5c-fe29-11e2-84b6-34e1f30fc148'
2013-08-06 00:42:07,683 - INFO - pipeline.rsync_tools - running rsync for files: ['tr/484b6d5c-fe29-11e2-84b6-34e1f30fc148']
2013-08-06 00:42:08,233 - INFO - pipeline.pipeline.worker-11 - Waiting for jobs...
2013-08-06 00:42:09,510 - INFO - pipeline.pipeline.worker-4 - Rsyncing from repo ['LatticeConstantCubicEnergy_Zr_sc__T
E_107850120912_000', 'EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000', 'LatticeConstantCubicEnergy__TD_475411767
977_000', 'EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000', 'EAM_Dynamo__MD_120291908751_000']
2013-08-06 00:42:09,520 - INFO - pipeline.rsync_tools - running rsync for files: ['./te/LatticeConstantCubicEnergy_Zr_sc__T
E_107850120912_000', './mo/EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000', './td/LatticeConstantCubicEnergy__TD_475411767977
_000', './mo/EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000', './md/EAM_Dynamo__MD_120291908751_000']
2013-08-06 00:42:09,649 - INFO - pipeline.pipeline.worker-10 - Running (<Test(LatticeConstantCubicEnergy_Zr_sc__TE_10
7850120912_000)>,<Model(EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_000)>)
2013-08-06 00:42:09,685 - INFO - pipeline.compute - running <Test(LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_0
00)> with <Model(EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_000)>
2013-08-06 00:42:09,712 - INFO - pipeline.template - attempting to process <open file '/home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running4892d187-fe29-11e2-9ec3-34e1f30fc148__TE_107850120912_000/pipeline.stdin', mode 'r' at 0x3
57d540> for ('EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_000','LatticeConstantCubicEnergy_Zr_sc__TE_107850
120912_000')
2013-08-06 00:42:09,734 - INFO - pipeline.compute - launching run...
2013-08-06 00:42:10,576 - INFO - pipeline.compute - Run completed in 0.8399848937988281 seconds
2013-08-06 00:42:10,982 - INFO - pipeline.compute - Copying the contents of /home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running4892d187-fe29-11e2-9ec3-34e1f30fc148__TE_107850120912_000/output to /home/openkim/openkim-repository/
tr/4892d187-fe29-11e2-9ec3-34e1f30fc148
2013-08-06 00:42:10,989 - INFO - pipeline.pipeline.worker-10 - Rsyncing results '4892d187-fe29-11e2-9ec3-34e1f30fc148'
2013-08-06 00:42:10,993 - INFO - pipeline.rsync_tools - running rsync for files: ['tr/4892d187-fe29-11e2-9ec3-34e1f30fc148']
2013-08-06 00:42:11,757 - INFO - pipeline.pipeline.worker-1 - Waiting for jobs...
2013-08-06 00:42:12,514 - INFO - pipeline.pipeline.worker-9 - Rsyncing from repo ['LatticeConstantCubicEnergy_Zr_sc__T
E_107850120912_000', 'kcc_meam_Fe_to_Ga__MO_145522277939_000', 'LatticeConstantCubicEnergy__TD_475411767977_000',
 'kcc_meam_Fe_to_Ga__MO_145522277939_000', 'kcc_meam_driver__MD_111291751625_000']
2013-08-06 00:42:12,529 - INFO - pipeline.rsync_tools - running rsync for files: ['./te/LatticeConstantCubicEnergy_Zr_sc__T
E_107850120912_000', './mo/kcc_meam_Fe_to_Ga__MO_145522277939_000', './td/LatticeConstantCubicEnergy__TD_475411767977_000', '/
./mo/kcc_meam_Fe_to_Ga__MO_145522277939_000', './md/kcc_meam_driver__MD_111291751625_000']
2013-08-06 00:42:12,608 - INFO - pipeline.pipeline.worker-4 - Running (<Test(LatticeConstantCubicEnergy_Zr_sc__TE_107
850120912_000)>,<Model(EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000)>)
2013-08-06 00:42:12,635 - INFO - pipeline.compute - running <Test(LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_0
00)> with <Model(EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000)>
2013-08-06 00:42:12,652 - INFO - pipeline.template - attempting to process <open file '/home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running48caf0b8-fe29-11e2-8782-34e1f30fc148__TE_107850120912_000/pipeline.stdin', mode 'r' at 0x3
5725d0> for ('EAM_Dynamo_Zhou_Johnson_Zr__MO_103270551167_000','LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_
000')
2013-08-06 00:42:12,670 - INFO - pipeline.compute - launching run...
2013-08-06 00:42:13,150 - INFO - pipeline.compute - Run completed in 0.4803011417388916 seconds
2013-08-06 00:42:13,651 - INFO - pipeline.compute - Copying the contents of /home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running48caf0b8-fe29-11e2-8782-34e1f30fc148__TE_107850120912_000/output to /home/openkim/openkim-repository/
tr/48caf0b8-fe29-11e2-8782-34e1f30fc148
2013-08-06 00:42:13,661 - INFO - pipeline.pipeline.worker-4 - Rsyncing results '48caf0b8-fe29-11e2-8782-34e1f30fc148'
2013-08-06 00:42:13,667 - INFO - pipeline.rsync_tools - running rsync for files: ['tr/48caf0b8-fe29-11e2-8782-34e1f30fc148']
2013-08-06 00:42:14,319 - INFO - pipeline.pipeline.worker-10 - Waiting for jobs...
2013-08-06 00:42:15,308 - INFO - pipeline.pipeline.worker-8 - Rsyncing from repo ['LatticeConstantCubicEnergy_Zr_sc__T
E_107850120912_000', 'model_YSZ_PF_Dipole__MO_394669891912_000', 'LatticeConstantCubicEnergy__TD_475411767977_000
', 'model_YSZ_PF_Dipole__MO_394669891912_000']
2013-08-06 00:42:15,317 - INFO - pipeline.rsync_tools - running rsync for files: ['./te/LatticeConstantCubicEnergy_Zr_sc__T
E_107850120912_000', './mo/model_YSZ_PF_Dipole__MO_394669891912_000', './td/LatticeConstantCubicEnergy__TD_475411767977_000',
'./mo/model_YSZ_PF_Dipole__MO_394669891912_000']
2013-08-06 00:42:15,410 - INFO - pipeline.pipeline.worker-9 - Running (<Test(LatticeConstantCubicEnergy_Zr_sc__TE_107
850120912_000)>,<Model(kcc_meam_Fe_to_Ga__MO_145522277939_000)>)
2013-08-06 00:42:15,426 - INFO - pipeline.compute - running <Test(LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_0
00)> with <Model(kcc_meam_Fe_to_Ga__MO_145522277939_000)>
2013-08-06 00:42:15,434 - INFO - pipeline.template - attempting to process <open file '/home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running4901de51-fe29-11e2-af15-34e1f30fc148__TE_107850120912_000/pipeline.stdin', mode 'r' at 0x3
57d270> for ('kcc_meam_Fe_to_Ga__MO_145522277939_000','LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_000')
2013-08-06 00:42:15,446 - INFO - pipeline.compute - launching run...
2013-08-06 00:42:17,134 - INFO - pipeline.compute - Run completed in 1.6879761219024658 seconds
2013-08-06 00:42:17,507 - INFO - pipeline.pipeline.worker-4 - Waiting for jobs...
2013-08-06 00:42:17,529 - INFO - pipeline.compute - Copying the contents of /home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running4901de51-fe29-11e2-af15-34e1f30fc148__TE_107850120912_000/output to /home/openkim/openkim-repository/
tr/4901de51-fe29-11e2-af15-34e1f30fc148
2013-08-06 00:42:17,537 - INFO - pipeline.pipeline.worker-9 - Rsyncing results '4901de51-fe29-11e2-af15-34e1f30fc148'
2013-08-06 00:42:17,542 - INFO - pipeline.rsync_tools - running rsync for files: ['tr/4901de51-fe29-11e2-af15-34e1f30fc148']
2013-08-06 00:42:18,321 - INFO - pipeline.pipeline.worker-8 - Running (<Test(LatticeConstantCubicEnergy_Zr_sc__TE_107
850120912_000)>,<Model(model_YSZ_PF_Dipole__MO_394669891912_000)>)
2013-08-06 00:42:18,338 - INFO - pipeline.compute - running <Test(LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_0
00)> with <Model(model_YSZ_PF_Dipole__MO_394669891912_000)>
2013-08-06 00:42:18,348 - INFO - pipeline.template - attempting to process <open file '/home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running49383cd4-fe29-11e2-8fe2-34e1f30fc148__TE_107850120912_000/pipeline.stdin', mode 'r' at 0x3
57d780> for ('model_YSZ_PF_Dipole__MO_394669891912_000','LatticeConstantCubicEnergy_Zr_sc__TE_107850120912_000')
2013-08-06 00:42:18,361 - INFO - pipeline.compute - launching run...
2013-08-06 00:42:18,990 - INFO - pipeline.compute - Run completed in 0.6283760070800781 seconds
2013-08-06 00:42:19,381 - INFO - pipeline.compute - Copying the contents of /home/openkim/openkim-repository/te/LatticeConstantCubicEnergy_Zr_sc_running49383cd4-fe29-11e2-8fe2-34e1f30fc148__TE_107850120912_000/output to /home/openkim/openkim-repository/
tr/49383cd4-fe29-11e2-8fe2-34e1f30fc148
2013-08-06 00:42:19,391 - INFO - pipeline.pipeline.worker-8 - Rsyncing results '49383cd4-fe29-11e2-8fe2-34e1f30fc148'
2013-08-06 00:42:19,396 - INFO - pipeline.rsync_tools - running rsync for files: ['tr/49383cd4-fe29-11e2-8fe2-34e1f30fc148']
2013-08-06 00:42:21,023 - INFO - pipeline.pipeline.worker-9 - Waiting for jobs...
2013-08-06 00:42:22,917 - INFO - pipeline.pipeline.worker-8 - Waiting for jobs...
```

Test Result - TE_156715955670_000-and-MO_123629422045_000

Model	MO_123629422045_000
Test	TE_156715955670_000

Files

Files

- kim.log
- kimspec.ini
- pipeline.processed.stdin
- pipeline.stderr
- pipeline.stdout
- results.yaml

```
---
crystal-structure:
  a:
    si-unit: m
    si-value: 4.03209980494e-10
    source-unit: angstrom
    source-value: 4.03209980494
  alpha:
    si-unit: rad
    si-value: 1.5707963267949
    source-unit: degrees
    source-value: 90
  b:
    si-unit: m
    si-value: 4.03209980494e-10
    source-unit: angstrom
    source-value: 4.03209980494
  beta:
    si-unit: rad
    si-value: 1.5707963267949
    source-unit: degrees
    source-value: 90
  c:
    si-unit: m
    si-value: 4.03209980494e-10
    source-unit: angstrom
    source-value: 4.03209980494
  gamma:
    si-unit: rad
    si-value: 1.5707963267949
    source-unit: degrees
    source-value: 90
  kim-ns: https://openkim.org/ns/openkim#primitive.crystal-structure
  short-name:
  - fcc
  space-group: Fm-3m
  wyckoff-site:
  - code: 4a
    fract-x:
      si-unit: '1'
      si-value: 0.0
      source-unit: 1
      source-value: 0
    fract-y:
      si-unit: '1'
      si-value: 0.0
      source-unit: 1
      source-value: 0
    fract-z:
      si-unit: '1'
      si-value: 0.0
      source-unit: 1
      source-value: 0
    set-or-measured: set
    species: Al
kim-template-pattern-comment: Using template pattern "Equilibrium Crystal Structure
  - 2013-04-24" as documented at https://openkim.org/cite/#openkim.org,2013-04-24:template-pattern/equilibrium-crystal-structure
kim-template-tags:
- equilibrium-crystal-structure
nvt:
  kim-ns: https://openkim.org/ns/openkim#primitive.equilibrium-ensemble-nvt
  temperature:
    si-unit: K
    si-value: 0.0
    source-unit: K
    source-value: 0
---
crystal-structure:
  a:
    si-unit: m
    si-value: 4.03209980494e-10
    source-unit: angstrom
    source-value: 4.03209980494
  alpha:
    si-unit: rad
    si-value: 1.5707963267949
    source-unit: degrees
    source-value: 90
  b:
    si-unit: m
    si-value: 4.03209980494e-10
    source-unit: angstrom
    source-value: 4.03209980494
  beta:
    si-unit: rad
    si-value: 1.5707963267949
    source-unit: degrees
    source-value: 90
  c:
    si-unit: m
    si-value: 4.03209980494e-10
    source-unit: angstrom
    source-value: 4.03209980494
  gamma:
    si-unit: rad
    si-value: 1.5707963267949
    source-unit: degrees
    source-value: 90
  kim-ns: https://openkim.org/ns/openkim#primitive.crystal-structure
  short-name:
  - fcc
  space-group: Fm-3m
  wyckoff-site:
  - code: 4a
    fract-x:
      si-unit: '1'
      si-value: 0.0
      source-unit: 1
      source-value: 0
    fract-y:
      si-unit: '1'
      si-value: 0.0
      source-unit: 1
      source-value: 0
    fract-z:
      si-unit: '1'
      si-value: 0.0
      source-unit: 1
      source-value: 0
    set-or-measured: set
    species: Al
energy:
  kim-ns: https://openkim.org/ns/openkim#primitive.cohesive-energy
  si-unit: m2.kg.s-2
  si-value: 5.38331582974528e-19
  source-unit: eV
  source-value: 3.36000000059
kim-template-pattern-comment: Using template pattern "Basic Cohesive Energy - 2013-04-24"
  as documented at https://openkim.org/cite/#openkim.org,2013-04-24:template-pattern/basic-cohesive-energy
kim-template-tags:
- cohesive-energy
nvt:
  kim-ns: https://openkim.org/ns/openkim#primitive.equilibrium-ensemble-nvt
  temperature:
    si-unit: K
    si-value: 0.0
    source-unit: K
    source-value: 0
```

Example queries (click to try)

Get all jobs that are currently running	Get all test drivers in the database	Get all fcc Al lattice constants and the model than 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

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')

map

1

A JavaScript function that operates to on the map portion of map-reduce. For more information, check the docs

reduce

1

A JavaScript function that operates to on the reduce portion of map-reduce. For more information, check the docs

database obj

Database you want, valid options are [obj, tr, vr, er, rd, job, log, agent]

skip [skip]

How many you want to skip, relevant if ordered

sort [sort]

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

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.

limit 3

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

flatten ☐

Whether or not to flatten the keys in the dictionary

Submit

OpenKIM Visualization

Atomic Configurations —

Description:
Atomic configuration visualizations powered by JSmol.

Functionality:
- Displays 3D crystal structure and surface test results from the knowledgebase.
- Allows user to capture a snapshot for later use.

Test Ext. ID:

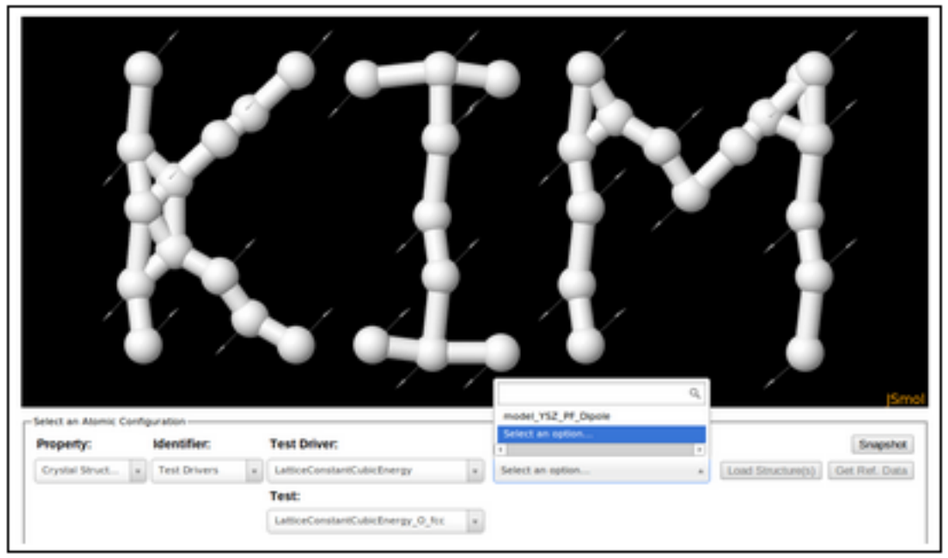
Model Ext. ID:

Test Driver Ext.ID:

Model Driver Ext. ID:

Property: Select a property...

Launch!



Click to launch with defaults...

Lattice Constant Scatter Plot +

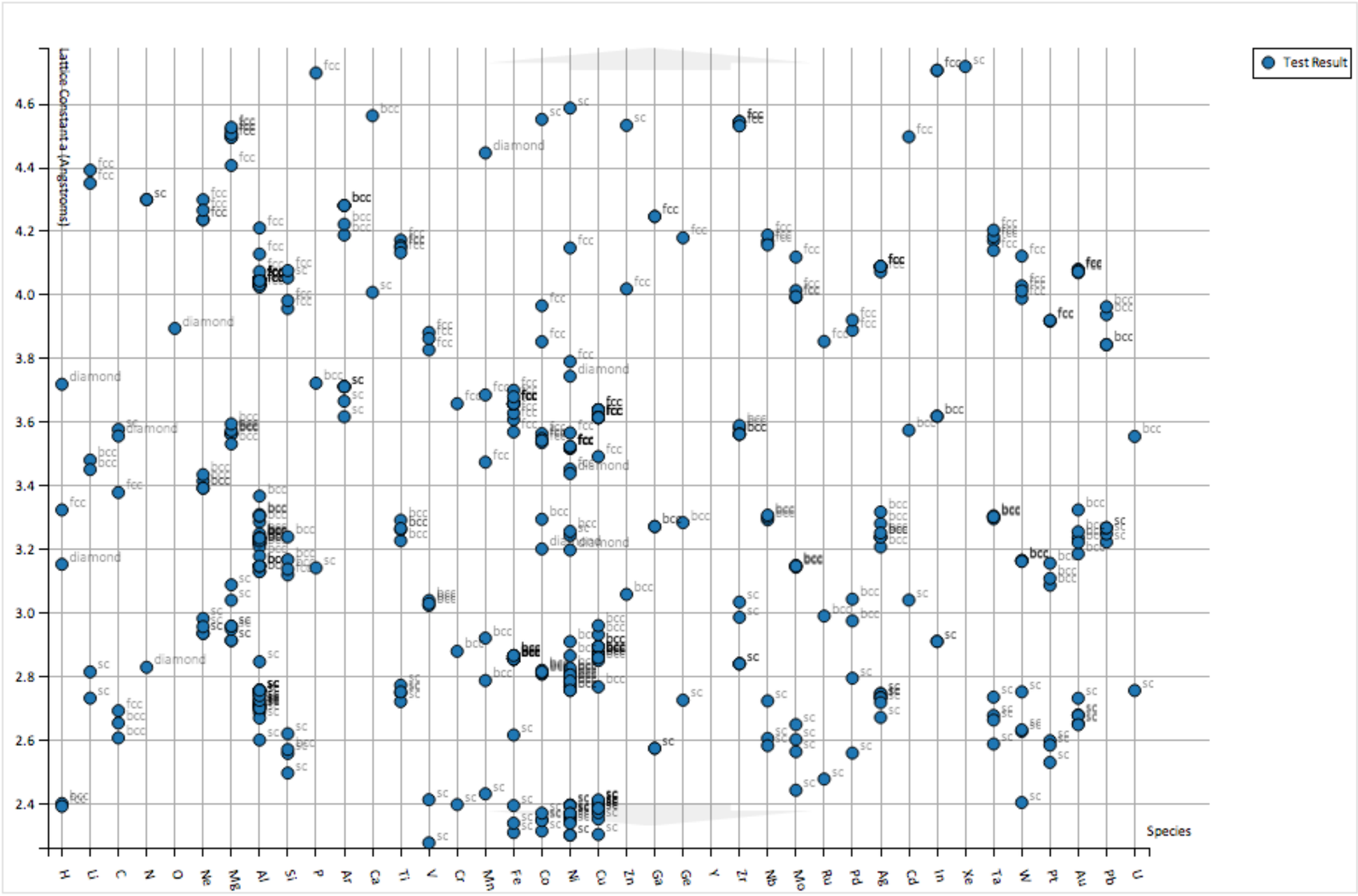
Cohesive Energy Scatter Plot +

Surface Energy Scatter Plot +

Bulk Modulus Scatter Plot +

Phonon Dispersion Relation Curve Plot +

OpenKIM Lattice Constant Plot



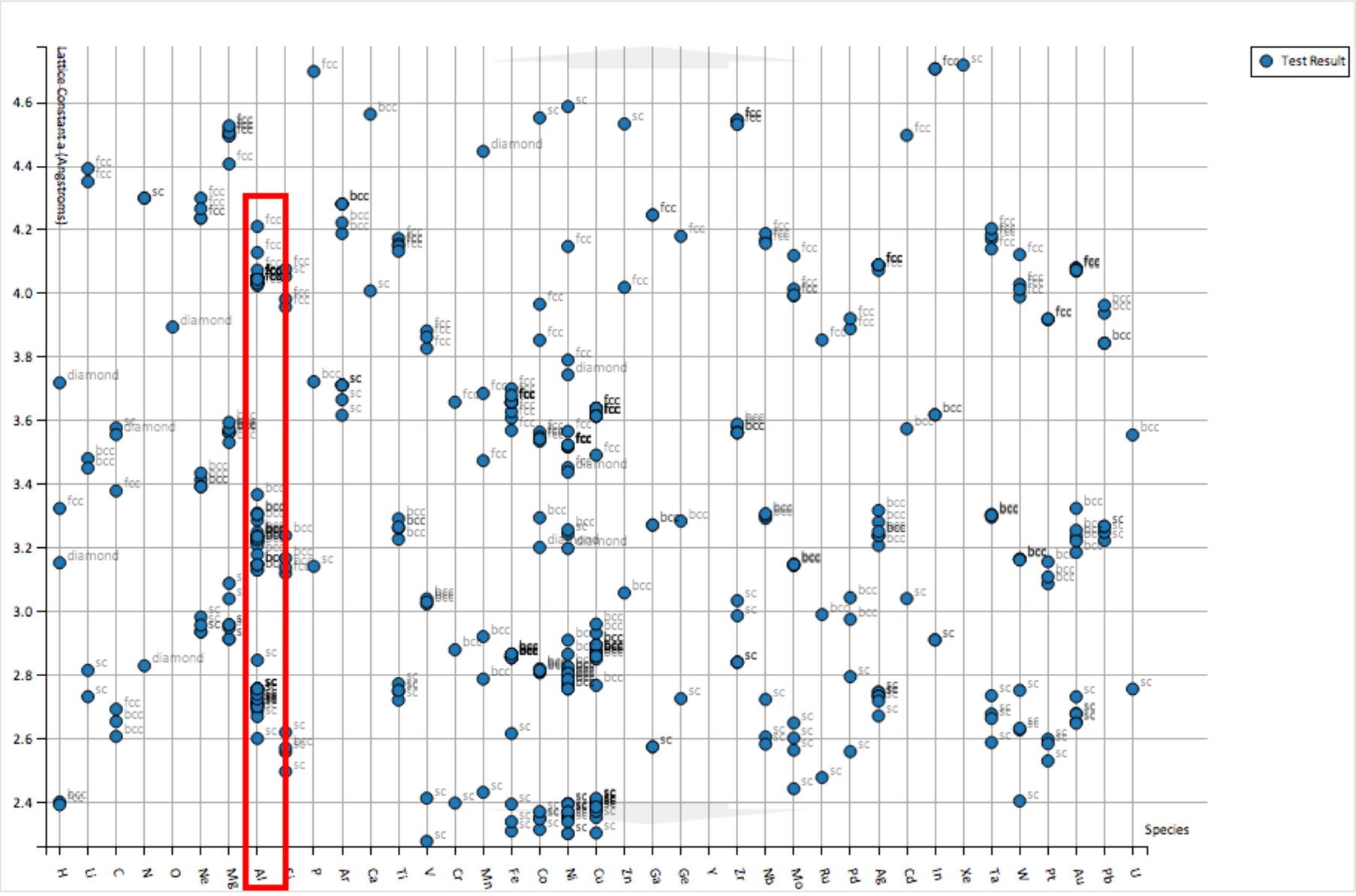
Query History:

```
16:19:52 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"rd"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"rd"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 238 ms

16:19:52 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"tr"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"tr"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 1099 ms

Learn to query
```

OpenKIM Lattice Constant Plot



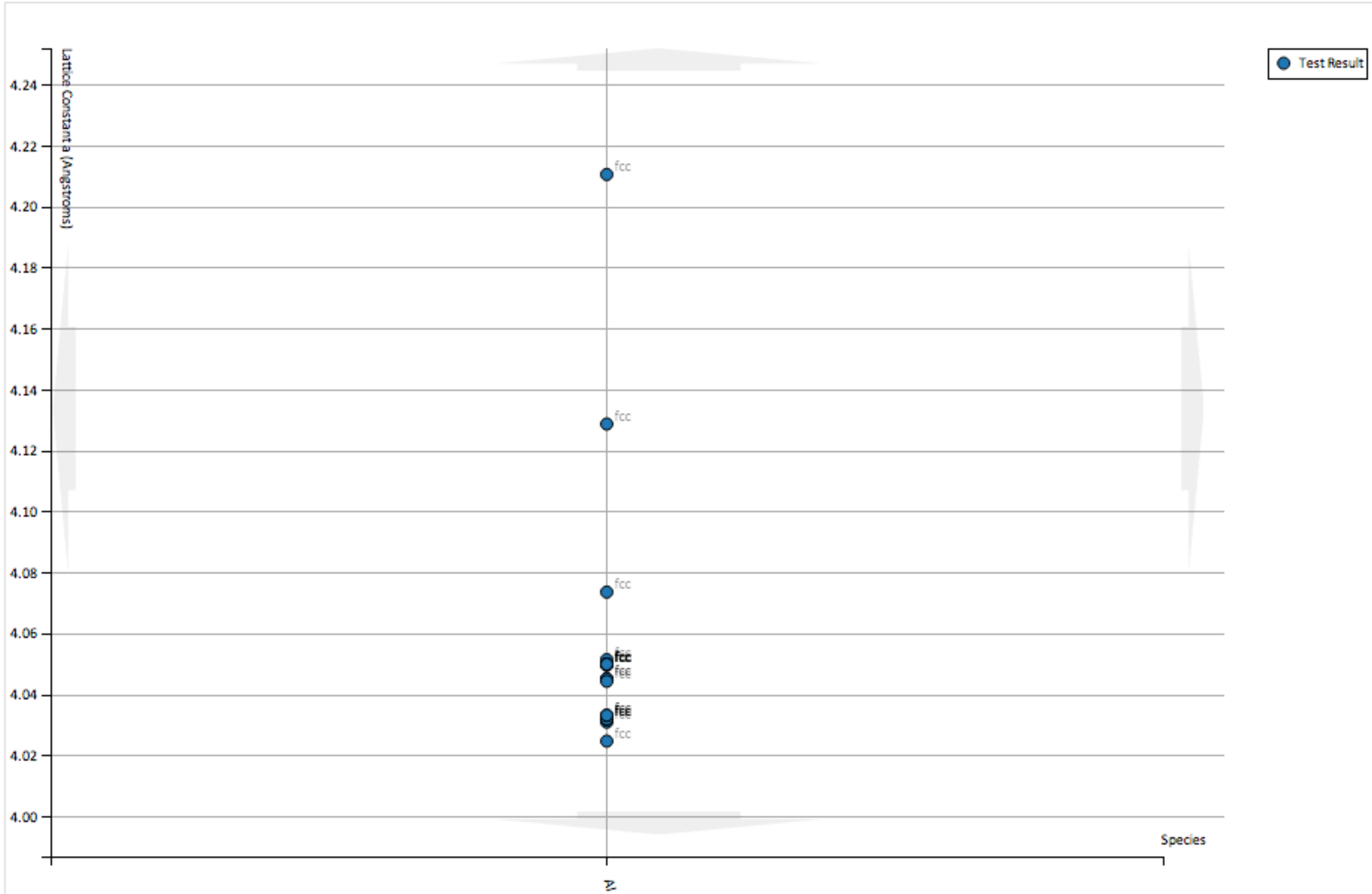
Query History:

```
16:19:52 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"rd"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"rd"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 238 ms

16:19:52 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"tr"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"tr"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 1099 ms

Learn to query
```

OpenKIM Lattice Constant Plot



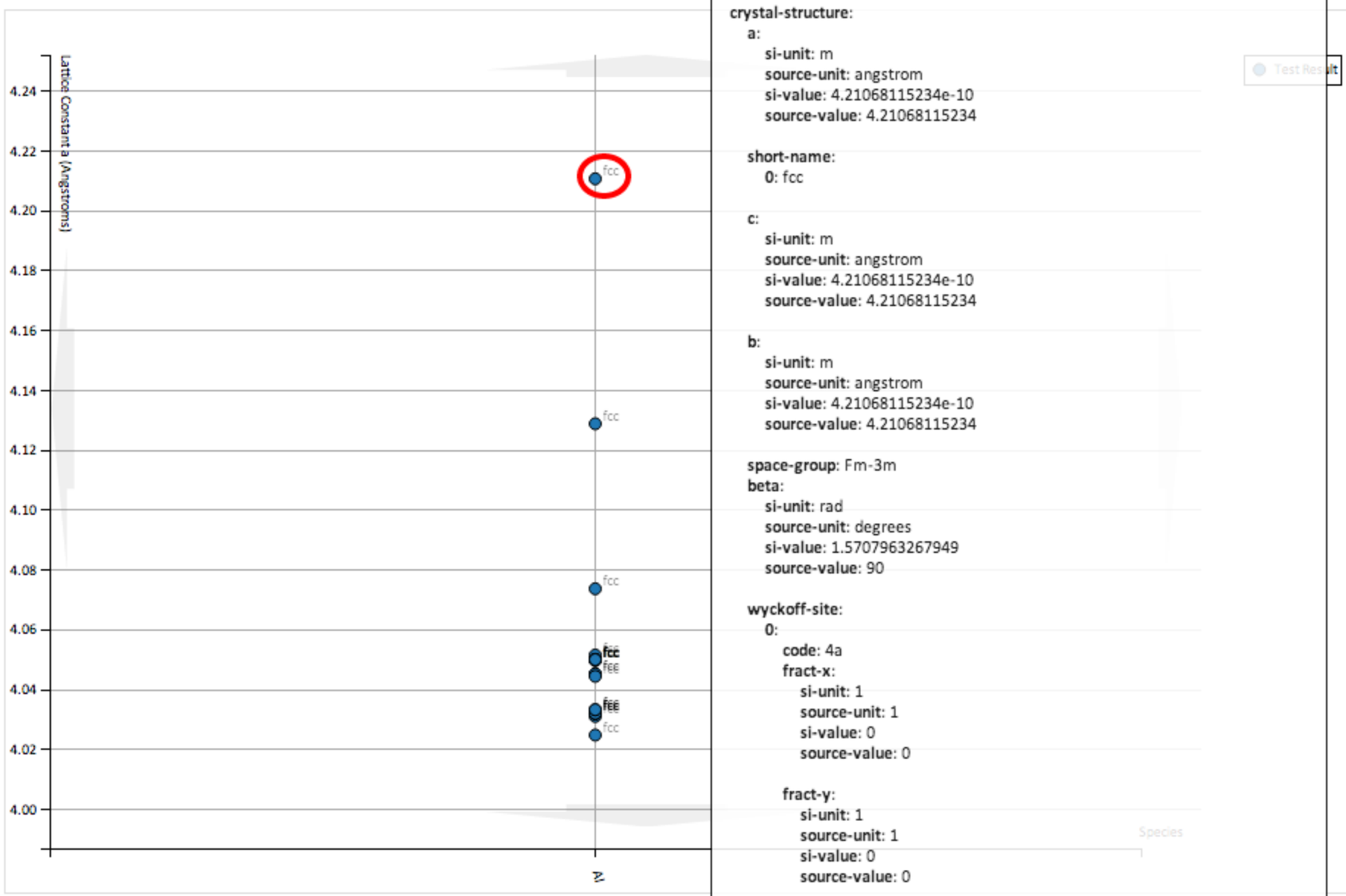
Query History:

```
16:19:52 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"rd"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"rd"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 238 ms

16:19:52 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"tr"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"tr"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 1099 ms

Learn to query
```

OpenKIM Lattice Constant Plot



Query History:

16:19:52 | URI: https://query.openkim.org/api
| Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"rd"}
| Database: data
| Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
| Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-structure","meta.type":"rd"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 238 ms

16:19:52 | URI: https://query.openkim.org/api
| Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"tr"}
| Database: data
| Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
| Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-structure","meta.type":"tr"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 1099 ms

Learn to query

Data Point Information

crystal-structure:
a:
si-unit: m
source-unit: angstrom
si-value: 4.21068115234e-10
source-value: 4.21068115234

short-name:
0: fcc

c:
si-unit: m
source-unit: angstrom
si-value: 4.21068115234e-10
source-value: 4.21068115234

b:
si-unit: m
source-unit: angstrom
si-value: 4.21068115234e-10
source-value: 4.21068115234

space-group: Fm-3m
beta:
si-unit: rad
source-unit: degrees
si-value: 1.5707963267949
source-value: 90

wyckoff-site:
0:
code: 4a
fract-x:
si-unit: 1
source-unit: 1
si-value: 0
source-value: 0

fract-y:
si-unit: 1
source-unit: 1
si-value: 0
source-value: 0

fract-z:
si-unit: 1
source-unit: 1
si-value: 0
source-value: 0

set-or-measured: set
species: Al

alpha:
si-unit: rad
source-unit: degrees
si-value: 1.5707963267949
source-value: 90

kim-ns: https://openkim.org/ns/openkim#primitive.crystal-structure
gamma:
si-unit: rad
source-unit: degrees
si-value: 1.5707963267949
source-value: 90

nvt:
kim-ns: https://openkim.org/ns/openkim#primitive.equilibrium-ensemble-nvt
temperature:
si-unit: K
source-unit: K
si-value: 0
source-value: 0

meta:
runner:
makeable: true
name: LatticeConstantCubicEnergy_Al_fcc
runner: true
shortcode: TE_156715955670
driver:
name: LatticeConstantCubicEnergy
shortcode: TD_475411767977
driver: true
kimcode: LatticeConstantCubicEnergy__TD_475411767977_000
version: 0
kimnum: 475411767977
path: td/LatticeConstantCubicEnergy__TD_475411767977_000
_id: LatticeConstantCubicEnergy__TD_475411767977_000
type: td
approved: true

approved: true
version: 0
kimnum: 156715955670
path: te/LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
_id: LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
type: te
kimcode: LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
subject: true

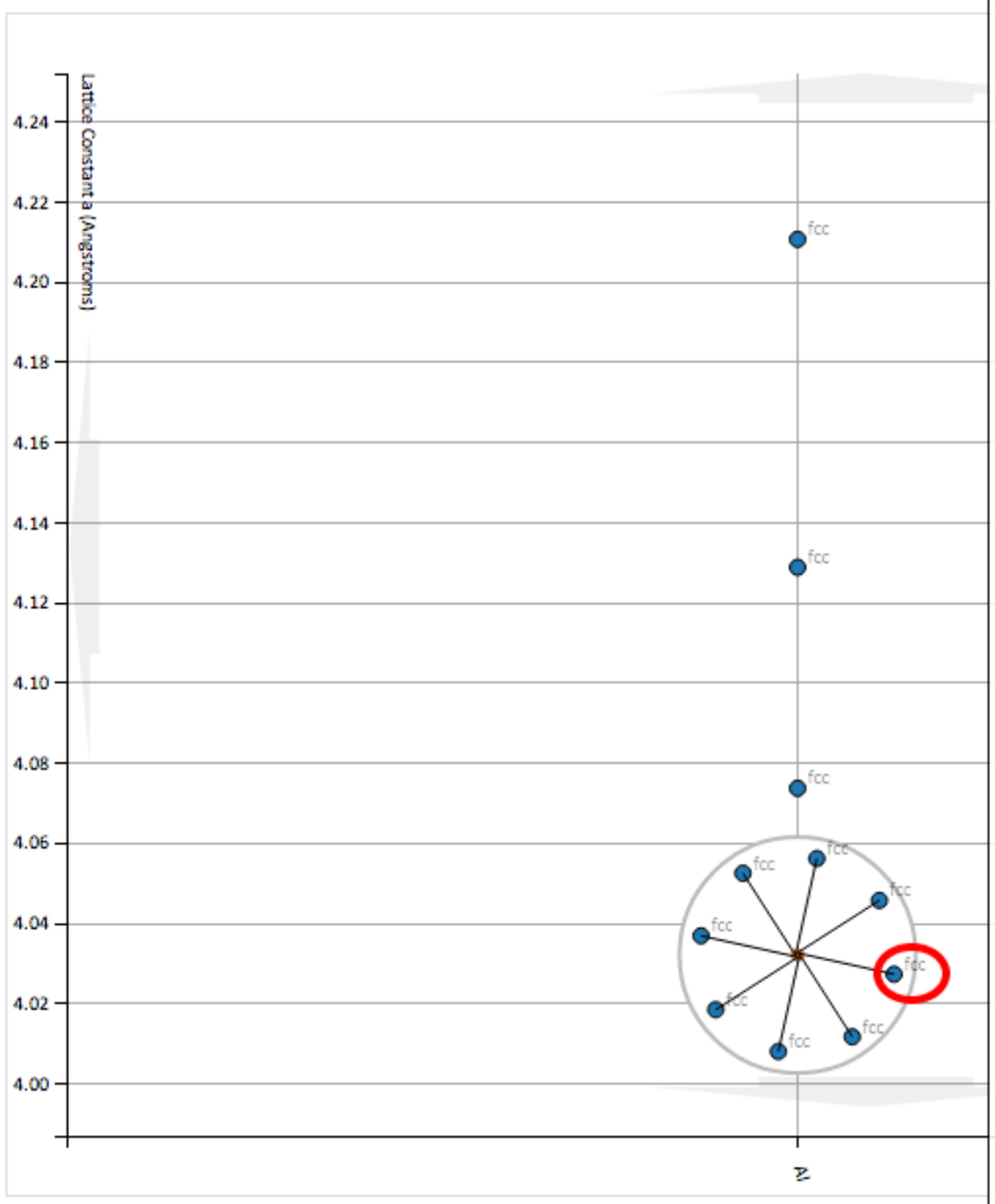
subject:
makeable: true
name: IMD_AlMnPd
shortcode: MO_878712978062
driver: false
approved: true
version: 0
kimnum: 878712978062
path: mo/IMD_AlMnPd__MO_878712978062_000
_id: IMD_AlMnPd__MO_878712978062_000
type: mo
kimcode: IMD_AlMnPd__MO_878712978062_000
subject: true

_id:
$oid: 52003b02c54fa17cd3be0faa

type: Test Result
species: Al

More details | Close

OpenKIM Lattice Constant Plot



Query History:

```
16:26:39 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"rd"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"rd"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 80 ms

16:26:39 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"tr"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"tr"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 1011 ms

16:26:33 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"rd","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"rd","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}&fields=
{"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 463 ms

16:26:33 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"tr","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"tr","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}&fields=
{"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 479 ms

16:19:52 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"equilibrium-crystal-structure","meta.type":"rd"}
         | Database: data
         | Fields: {"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"equilibrium-crystal-
structure","meta.type":"rd"}&fields={"crystal-structure":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 238 ms

Learn to query
```

Data Point Information

crystal-structure:
  a:
    si-unit: m
    source-unit: angstrom
    si-value: 4.03209980494e-10
    source-value: 4.03209980494

  short-name:
    0: fcc

  c:
    si-unit: m
    source-unit: angstrom
    si-value: 4.03209980494e-10
    source-value: 4.03209980494

  b:
    si-unit: m
    source-unit: angstrom
    si-value: 4.03209980494e-10
    source-value: 4.03209980494

  space-group: Fm-3m
  beta:
    si-unit: rad
    source-unit: degrees
    si-value: 1.5707963267949
    source-value: 90

  wyckoff-site:
    0:
      code: 4a
      fract-x:
        si-unit: 1
        source-unit: 1
        si-value: 0
        source-value: 0

      fract-y:
        si-unit: 1
        source-unit: 1
        si-value: 0
        source-value: 0

      fract-z:
        si-unit: 1
        source-unit: 1
        si-value: 0
        source-value: 0

      set-or-measured: set
      species: Al

  alpha:
    si-unit: rad
    source-unit: degrees
    si-value: 1.5707963267949
    source-value: 90

  kim-ns: https://openkim.org/ns/openkim#primitive.crystal-structure
  gamma:
    si-unit: rad
    source-unit: degrees
    si-value: 1.5707963267949
    source-value: 90

  nvt:
    kim-ns: https://openkim.org/ns/openkim#primitive.equilibrium-ensemble-nvt
    temperature:
      si-unit: K
      source-unit: K
      si-value: 0
      source-value: 0

  meta:
    runner:
      makeable: true
      name: LatticeConstantCubicEnergy_Al_fcc
      runner: true
      shortcode: TE_156715955670
      driver:
        name: LatticeConstantCubicEnergy
        shortcode: TD_475411767977
        driver: true
        kimcode: LatticeConstantCubicEnergy__TD_475411767977_000
        version: 0
        kimnum: 475411767977
        path: td/LatticeConstantCubicEnergy__TD_475411767977_000
        _id: LatticeConstantCubicEnergy__TD_475411767977_000
        type: td
        approved: true

      approved: true
      version: 0
      kimnum: 156715955670
      path: te/LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
      _id: LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
      type: te
      kimcode: LatticeConstantCubicEnergy_Al_fcc__TE_156715955670_000
      subject: true

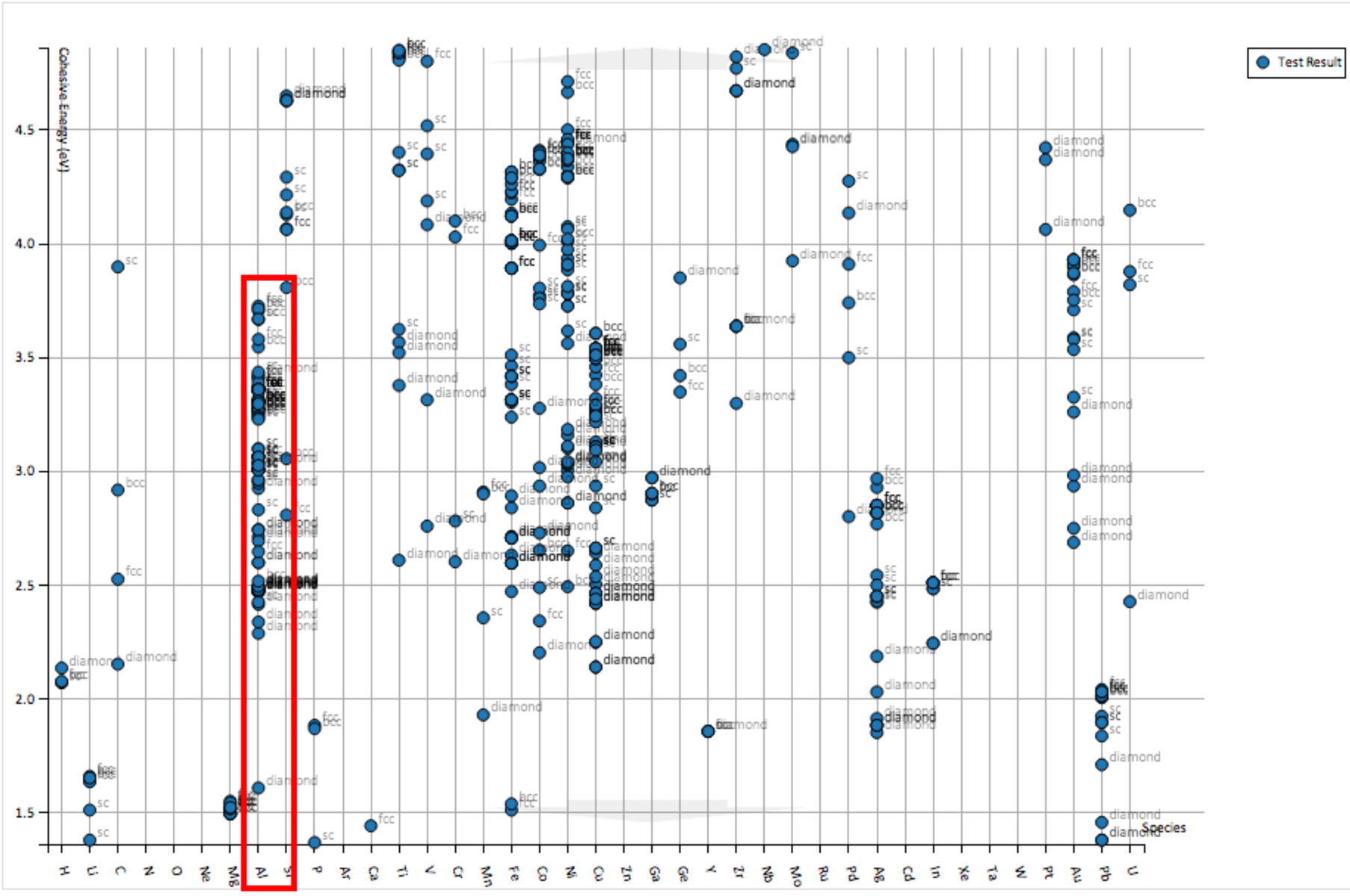
    subject:
      makeable: true
      name: EAM_Dynamo_Ercolessi_Adams_Al
      shortcode: MO_123629422045
      driver: false
      approved: true
      version: 0
      kimnum: 123629422045
      path: mo/EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000
      _id: EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000
      type: mo
      kimcode: EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000
      subject: true

_id:
  $oid: 52003ad7c54fa17cd3be0e9f

type: Test Result
species: Al

More details | Close

OpenKIM Cohesive Energy Plot

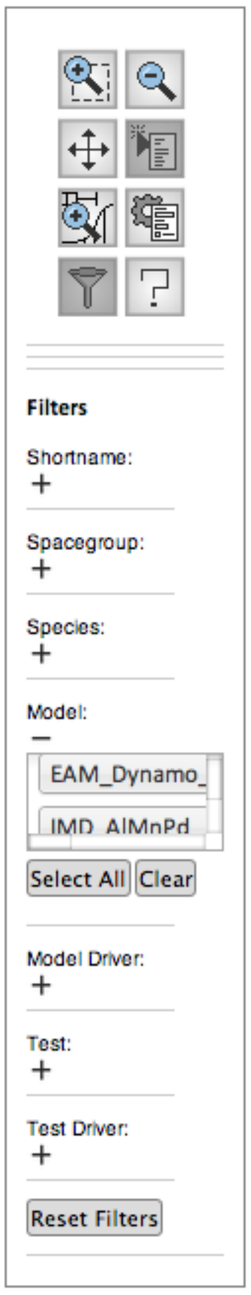


Query History:

```
16:34:02 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"cohesive-energy","meta.type":"rd"}
         | Database: data
         | Fields: {"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"cohesive-
energy","meta.type":"rd"}&fields={"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 221 ms

16:34:02 | URI: https://query.openkim.org/api
         | Query: {"kim-template-tags":"cohesive-energy","meta.type":"tr"}
         | Database: data
         | Fields: {"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
         | Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"cohesive-
energy","meta.type":"tr"}&fields={"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 1116 ms

Learn to query
```



OpenKIM Cohesive Energy Plot

Query History:

22:09:25 | URI: https://query.openkim.org/api
| Query: {"kim-template-tags":"cohesive-energy","meta.type":"rd","$or" : [{"meta.subject.kimcode":"IMD_AlMnPd__MO_878712978062_000"},{"meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}]}
| Database: data
| Fields: {"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
| Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"cohesive-energy","meta.type":"rd","$or" : [{"meta.subject.kimcode":"IMD_AlMnPd__MO_878712978062_000"},{"meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}]}&fields={"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 188 ms

22:09:25 | URI: https://query.openkim.org/api
| Query: {"kim-template-tags":"cohesive-energy","meta.type":"tr","$or" : [{"meta.subject.kimcode":"IMD_AlMnPd__MO_878712978062_000"},{"meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}]}
| Database: data
| Fields: {"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
| Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"cohesive-energy","meta.type":"tr","$or" : [{"meta.subject.kimcode":"IMD_AlMnPd__MO_878712978062_000"},{"meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}]}&fields={"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 587 ms

22:08:40 | URI: https://query.openkim.org/api
| Query: {"kim-template-tags":"cohesive-energy","meta.type":"rd","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}
| Database: data
| Fields: {"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
| Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"cohesive-energy","meta.type":"rd","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}&fields={"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 494 ms

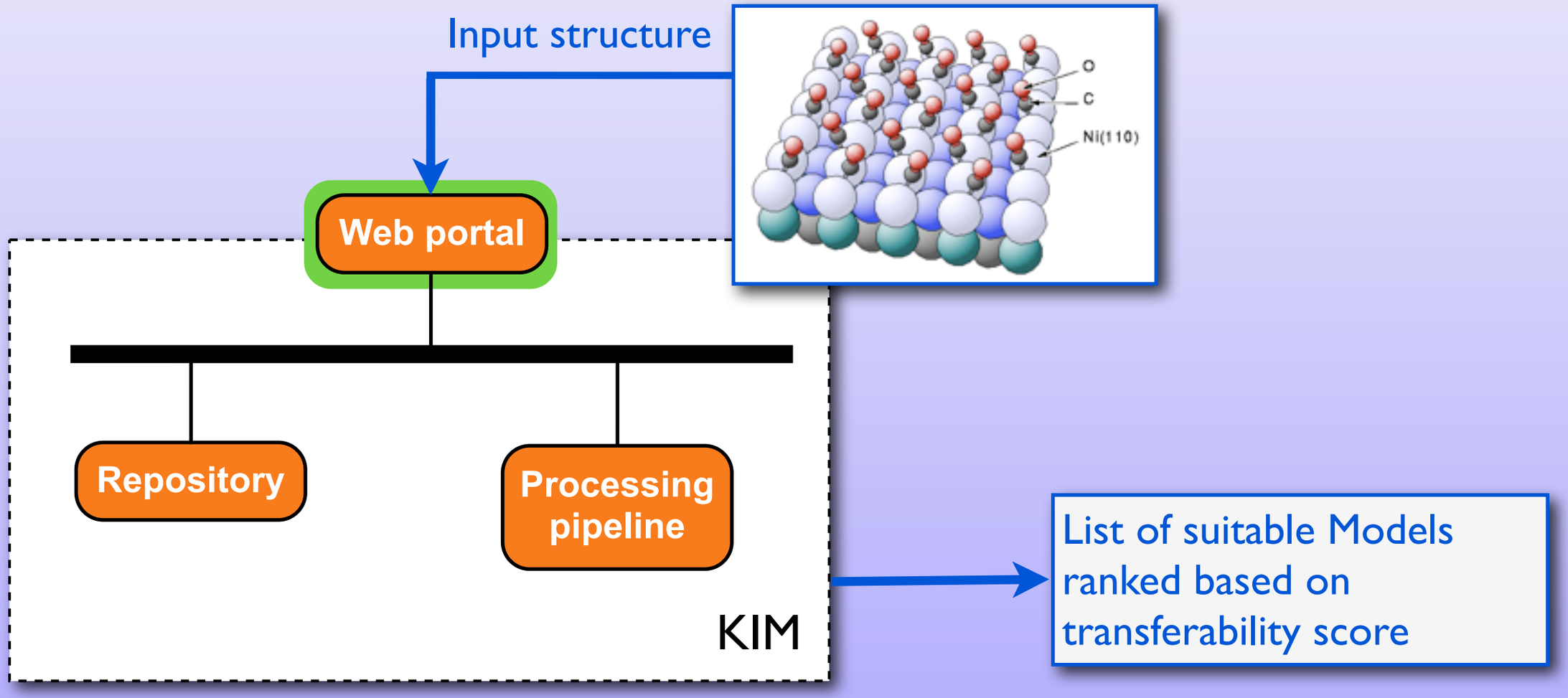
22:08:40 | URI: https://query.openkim.org/api
| Query: {"kim-template-tags":"cohesive-energy","meta.type":"tr","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}
| Database: data
| Fields: {"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
| Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"cohesive-energy","meta.type":"tr","meta.subject.kimcode":"EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_000"}&fields={"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 345 ms

22:07:34 | URI: https://query.openkim.org/api
| Query: {"kim-template-tags":"cohesive-energy","meta.type":"rd"}
| Database: data
| Fields: {"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
| Link: https://query.openkim.org/?database=data&query={"kim-template-tags":"cohesive-energy","meta.type":"rd"}&fields={"crystal-structure":1,"energy":1,"meta.runner":1,"meta.subject":1,"nvt":1}
Query took 229 ms

Learn to query

Interacting with KIM

Scenario IV: Finding an appropriate potential for a given application



KIM Organization

- KIM Inaugural Meeting held in San Diego, Feb 26-27, 2011
  - 63 participants from 7 countries
  - Many key model developers present
  - Major code developers present:
    - LAMMPS, iMD, GROMACS, SPaSM, DL_POLY
  - KIM Requirements Document defined and posted online (openKIM.org/requirements).

  - KIM organizational structure decided and voted on:
    - KIM Director: Ellad Tadmor (U. Minnesota)
    - KIM Editor: Ryan Elliott (U. Minnesota)
    - KIM Board: Mike Baskes (UCSD/LANL), Chandler Becker (NIST), Ronald Miller (Carleton U.), Susan Sinnott (U. Florida), Sadasivan Shankar (Intel), Aidan Thompson (Sandia)
  - 378 KIM Members (July 2013)

Starting the Snowball Rolling

- Current release: KIM API Version 1.2.1 (July 2013)

- The current focus of the KIM project is to modify as many existing interatomic potentials to conform to the KIM API.

- To facilitate this we are holding a series of

KIM Content Carnivals (KCC)

- Travel expenses, local housing and honorarium can be provided to participants.
- Participation by invitation only.
- Previous: Minneapolis (3/12), Aachen (8/12), Singapore (10/12)
- UPCOMING EVENTS:
  - None scheduled at this time but keep checking the website.

For more information: http://openKIM.org