

Model Upload Preparation Sheet

Uploading a new interatomic model to OpenKIM involves [filling in a form](#) with metadata about the model and any necessary parameter files in the appropriate format for that model type. Below is a description of all the input that will need to be provided. This is a fillable form. Make a copy of this document and fill it in for every model you plan to upload. You can then simply cut and paste into the online form as you perform the upload. If you have any questions, email support@openkim.org or post to the [OpenKIM Google Group](#).

Models in OpenKIM come in two flavors: *Portable Models (PMs)*, which can be used with any simulation code compatible with the KIM API standard, and *Simulator Models (SMs)*, which only work with a specific simulation code. PMs are identified by the Model Driver for their class, and SMs are identified by the simulation code (Simulator) and the potential's designation within that code. Uploading using a Model Driver is preferred when possible since the model will be usable in multiple codes and therefore have maximum exposure. (If you select to upload an SM for a potential type supported through a KIM Driver, you will be taken to a screen to select the KIM Driver.)

Each model uploaded to KIM is “owned” by whoever contributes it. This person can make changes to the information accompanying the model and is the contact point for it. To contribute a model, you have to be a KIM member. If you are not a KIM member, you can register here for free: <https://openkim.org/new-account>

The upload process is divided into different steps with different information required in each step. Depending on whether you are uploading a PM or SM, the required information can be different.

STEP 1: Define the type of model being uploaded.

- Is this a PM or SM (select one):

Portable Model (PM)

Simulator Model (SM)

- For a PM, the **KIM Model Driver**:

See the [list of KIM Drivers](#) for your options.

Example:

- `EAM_Dynamo__MD_120291908751_005` (this is the standard KIM driver for EAM potentials equivalent to the one implemented in LAMMPS).

- For an SM, the **Simulator and Potential**:

See the simulator documentation for available potential types (e.g. the [pair styles in LAMMPS](#)). (If the potential type is supported through a KIM Driver, you will be prompted to select a Driver.)

Example:

- `LAMMPS – meam/c` (this is the meam/c pair style implemented in LAMMPS).

STEP 2: Provide information and parameters for the model being uploaded.

Section 1

This section completes the definition of the model. This includes technical information that in most cases does not need to be changed. If you are unsure, make no changes.

- For a PM, no additional information is required.
- For an SM, the following information is required:
 - **Simulator Version** (*The latest version of the simulator with which this SM is known to have run correctly*)

Example:

- LAMMPS provides version information as a date, e.g. **22 Sep 2017**
- **Model Initialization** (*Commands passed to simulator to initialize the potential. In most cases the default should not be changed.*)
- **Model Definition** (*Commands passed to simulator to define the potential. In most cases the default should not be changed.*)
- **Run Compatibility** (*The types of tests and verification checks that the model is compatible with. In most cases the default should not be changed.*)
- **Units** (*specification of the units used by the potential. In most cases the default should not be changed.*)

Section 2

This section deals with the parameter files that define the atomic interactions in the model.

- **Parameter Filename(s):**

Assemble all required parameter file(s) in the appropriate format. The format can be determined by seeing the [documentation for the appropriate KIM Model Driver](#) or the documentation for the simulator (e.g. [LAMMPS pair style documentation](#)).

Section 3

This section deals with the species that the model supports.

- **Supported Species:**

This is the list of chemical elements that the model supports.

Example:

- Ni, Al

Section 4

This section deals with metadata related to the model. This information will be included in the digital object identifier (DOI) that will be assigned to the model when it is created. DOIs provide a persistent identifier for the model and are indexed by data aggregators like Google and Clarivate Analytics that owns Web of Science.

- **Author(s):**

Author(s) of this item. To be used in citing this model.

- **Title:**

This is a brief sentence (without an ending period) describing the potential. The KIM convention is to include the simulator (for an SM), type of potential, supported species, authors, year and version (which will always be "v000" for a new upload).

Examples:

- EAM potential (LAMMPS cubic hermite tabulation) for Al developed by Ercolessi and Adams (1994) v000
- LAMMPS ADP Potential for Ni developed by Mishin et al. (2005) v000

Description:

A short description of the model's key features including for example: type of model (pair potential, 3-body potential, EAM, etc.), modeled species (Ac, Ag, ..., Zr), intended purpose, origin, and so on. This can be based on the abstract of a journal article associated with the model.

- **Content Origin** (optional):

A description and/or web address to the online source where the model parameter files were obtained.

- **Content Other Location** (optional):

A description and/or web address(es) to other location(s) where the content is available.

- **Disclaimer** (optional):

A short statement of applicability which will accompany any results computed using it. A developer can use the disclaimer to inform users of the intended use of this model.

Examples:

- *By design, this potential is not expected to be accurate for geometries with extremely low coordination -- such as small molecules -- which were not included in the training set.*
- *This model is designed for two-dimensional (2D) monolayer molybdenum disulfide (MoS₂). It is not appropriate for bulk MoS₂ or other compounds of Mo and/or S.*

- **Source Citations** (optional)

Citations to journal publications that should be references when the uploaded model is used. This information is listed on the OpenKIM website and is also provided at run time when the model is used in a simulation code (e.g. in LAMMPS, see Citation of OpenKIM IMs in the [LAMMPS documentation](#)).

Citations are uploaded in [BibTex format](#). A separate BibTex file can be uploaded for each source or a single file containing all citations. Alternatively, the user can manually fill in the BibTex fields in the online form.

Use the space above to record the BibTex filename(s) or the actual citations if you plan to upload them manually.



- **Funding Information** (optional):

List of funding sources acknowledged for supporting the development of the model. The following information is associated with each funding source:

- **Funder Name** (required). *Name of the funding organization. This will be selected from a curated list at upload time.*
- **Award Number** (optional).
- **Award URI** (optional). *Website address to more information on the award.*
- **Award Title** (optional).

- **Distribution License:**

*The license under which the model parameter files are being made available. [A variety of open source and proprietary licenses](#) can be selected at upload time. The license recommended by OpenKIM as providing the best balance in protecting user rights and making the content accessible is the **Common Development and Distribution License Version 1.0 (CDDL-1.0)**.*