

JARVIS-FF

**Evaluation and comparison of classical
interatomic potentials**

What is JARVIS-FF?

JARVIS-FF is a **database** designed to help Molecular Dynamics and/or Monte Carlo users to **choose the classical empirical potential that is right for their simulational needs**.

At the moment the database consists of 3583 entries among **energetics** and **elastic property** calculations, and is currently being expanded to include **surface and defect-related properties** as well as **phonon**-related data. All properties are computed for **all empirical potentials available to LAMMPS users or deposited into the NIST Interatomic Potential Repository (IPR)**, and are compared to density functional theory (DFT) as well as to experimental data, where available.

The most notable characteristic of this database is its **easy-to-use web-interface** that has been designed expressly to **facilitate direct comparison between potentials**. This is accomplished through clear look-up tables that allow to compare at a glance the results from different potentials for the same or similar systems.

We greatly appreciate publicly available Pymatgen, Phonopy and ASE tools.

All data in the database, as well as all the metadata needed to reproduce the results are **available for download** from the website <http://www.ctcms.nist.gov/~knc6/periodic.html>

Methodology

1. **Structural data:** we downloaded all the available potentials from the NIST interatomic potential repository (IPR) and from LAMMPS itself (15May2015 version). For each element having at least a potential, we downloaded all the corresponding crystal structures from the Materials Project(link is external) (MP) database. We also downloaded all the energetics and mechanical properties data from MP for comparison purposes.
2. **High-throughput calculations:** The high-throughput setting of the LAMMPS jobs was done using the **Mpinterfaces** (<http://www.sciencedirect.com/science/article/pii/S0927025616302440>). Using such a framework, for each force field and structure we calculated the energetics and 21 distinct elastic constants using the script(link is external) provided in the LAMMPS distribution version 15May2015. Using the energetics information for each material, convex hull plot were drawn using the package provided in **Pymatgen** (script named PDPlotter.py). All the input and output data for the calculations were saved in zipped and JSON format files and are available on the website.
3. **User-interface:** The data is presented in an interactive periodic table format. The four major aspects of our web interface are as shown in Fig.1: first (panel a)) is the search box, where the user can type the element or element combination of interest. The interactive periodic table that appears as the web page is opened is shown in panel b). Here the user can input the query by simply clicking on the element or element combination of interest. Panel c) shows the header. The last panel (d) contains the actual data for all the quantities discussed in the header section. These data are interactive in nature, as, for instance, clicking on the “Calcs” tab downloads the zipped input and output files of the LAMMPS calculations

a)

b)

JARVIS for Force-fields

Search
Ni-Al
Refresh

Periodic table showing elements color-coded by groups.

c)

d)

JARVIS-ID	MPID	Formula	Energy/atom (eV)	C ₁₁ (GPa)	C ₁₂ (GPa)	C ₁₃ (GPa)	C ₂₂ (GPa)	C ₂₃ (GPa)	C ₃₃ (GPa)	C ₄₄ (GPa)	C ₅₅ (GPa)	C ₆₆ (GPa)	B ₁ (GPa)	G ₁ (GPa)	Energy_hull (DFT)	Force-field
Calc-129	mp-1057	Ni ₂ Al ₃	-4.16	204.0	204.0	228.8	112.3	74.1	74.1	46.1	46.1	45.9	128.6	52.7	0.0	Mohan-Ni-Al-2009-asm.alloy
Calc-726	mp-1057	Ni ₂ Al ₃	-3.94	160.5	160.3	227.9	80.0	26.0	25.9	25.1	25.1	40.2	90.3	45.9	0.0	Offield-Comb3-NiAlD
Calc-836	mp-1057	Ni ₂ Al ₃	-4.13	270.3	270.3	334.6	192.0	140.3	140.3	52.2	52.2	39.1	202.3	55.5	0.0	NiAl ₂ -yes-asm.alloy
Calc-113	mp-1057	Ni ₂ Al ₃	-4.17	217.5	217.5	236.4	116.6	84.0	84.0	68.1	68.1	30.5	137.8	65.1	0.0	NiAl ₂ -C-asm.alloy
Calc-1066	mp-1057	Ni ₂ Al ₃	-4.16	204.1	204.1	228.9	112.3	74.1	74.1	46.1	46.1	45.9	128.7	52.7	0.0	Mohan-Ni-Al-Ce-2013-asm.alloy

Left sidebar menu:

- data
- inelastic
- init
- log
- potential
- restart.equil

Bottom panel showing a 3D crystal structure visualization of Ni₂Al₃ with a legend for Structure Type (Conventional Unitcell, Facecent, Defect) and Space Filling (Polyhedra).

Right panel showing a search result for "Mohan-Ni-Al-2009-asm.alloy" with a checkbox to select it.

Fig.1: Main components of the web user interface

Capabilities

- ❑ **Raw data** for energetics, elastic properties, surface and defect-related properties, phonons
- ❑ **Derived Quantities:** Thanks to the high-throughput nature of Jarvis, the user has a multitude of data available for the material/structure of interest. Interesting derived quantities can then be obtained, as, for instance, **convex-hull plots** that are used to know the phase stability of a material on the basis of composition and energetics information. The scripts for plotting multi-component convex-hull plot is provided at the Github page.

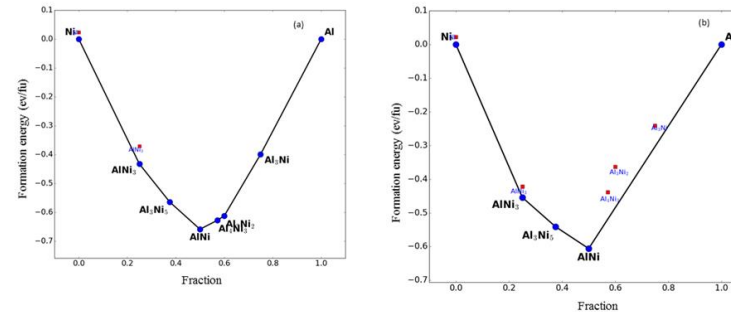
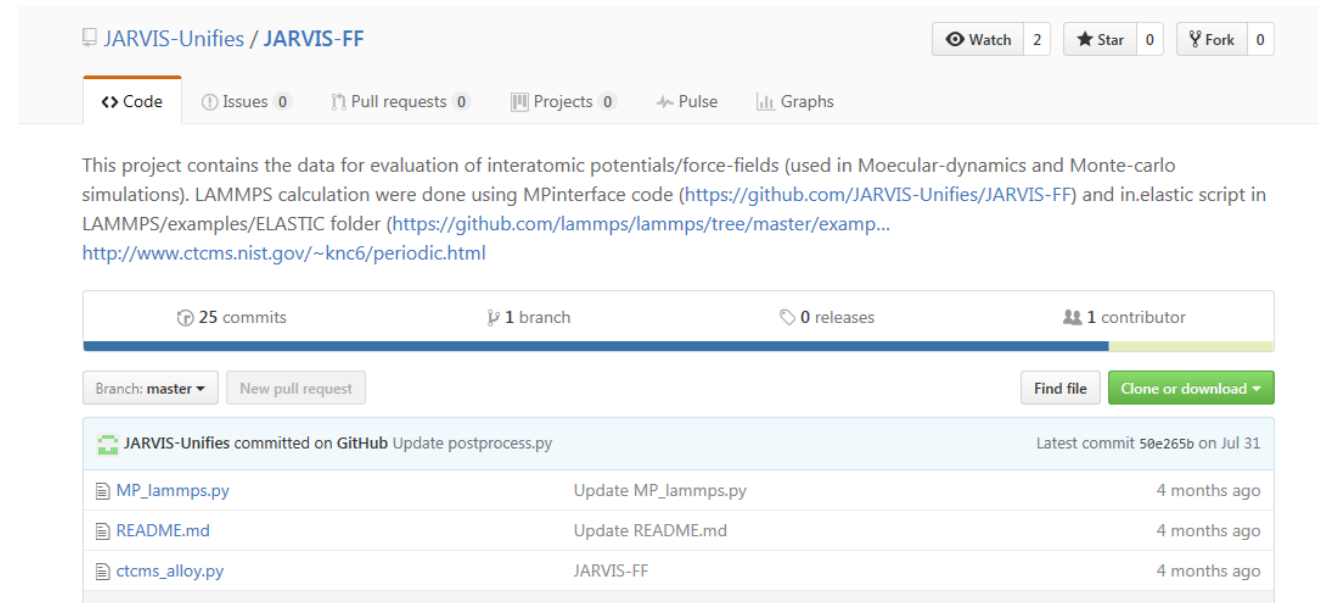


Figure 2. Convex hull plot for Ni-Al system using a) DFT (MP data), b) Force-field (Mishin Ni-Al potential).

- ❑ **Data analytics:** Data analytics tools provide the opportunity to determine correlations in data sets that can illuminate the accuracy of predictions and the flexibility of underlying models. As an example, to investigate if there are any trends in the elastic properties predicted by the various potentials, we used the data in Jarvis to perform a **principal-component analysis** on the relative errors of the predicted elastic constants compared to experimental data experimental data for the four FCC elements with the largest number of available potentials, i.e. Al, Cu, Ni, and Ag.

Code availability

- ❖ JARVIS-FF is written in python and it is **publicly available on Github** (<https://github.com/JARVIS-Unifies/JARVIS-FF>).



The screenshot shows the GitHub repository for JARVIS-Unifies/JARVIS-FF. At the top, it displays the repository name and navigation links for Watch (2), Star (0), and Fork (0). Below this, there are tabs for Code, Issues (0), Pull requests (0), Projects (0), Pulse, and Graphs. The main content area states: "This project contains the data for evaluation of interatomic potentials/force-fields (used in Molecular-dynamics and Monte-carlo simulations). LAMMPS calculation were done using MPinterface code (<https://github.com/JARVIS-Unifies/JARVIS-FF>) and in.elastic script in LAMMPS/examples/ELASTIC folder (<https://github.com/lammps/lammps/tree/master/examp...>) <http://www.ctcms.nist.gov/~knc6/periodic.html>". Below this, statistics show 25 commits, 1 branch, 0 releases, and 1 contributor. A bar chart shows the commit history. At the bottom, there is a table of recent commits:

Commit	Message	Time
JARVIS-Unifies committed on GitHub	Update postprocess.py	Latest commit 50e265b on Jul 31
MP_lammps.py	Update MP_lammps.py	4 months ago
README.md	Update README.md	4 months ago
ctcms_alloy.py	JARVIS-FF	4 months ago

Pre/Post Processing Tools for use with LAMMPS

This page gives pointers to various software tools and data repositories which can be used in conjunction with LAMMPS.

Speaking for the LAMMPS developers, we think these kinds of tools, whether free-ware or commercial software, can be very useful. They extend the scope of problems and its ease of use. We are happy to "advertise" such tools here, so that people can try them out. Send us an email if you want to add your software or tools that you use to

[GUI and Analysis Software](#) - 3rd-party commercial software that wraps LAMMPS

- [Materials Design, Inc.](#)
- [Scienomics](#)
- [Scifes Inc](#)
- [XenoView](#)

[Molecular Builders](#) - free software to build molecular inputs for LAMMPS

- [Enhanced Monte Carlo](#)
- [Moltemplate](#)
- [VMD TopoTools](#)
- [Avogadro](#)
- [Packmol](#)
- [Atomsk](#)
- [OCTA and J-OCTA](#)

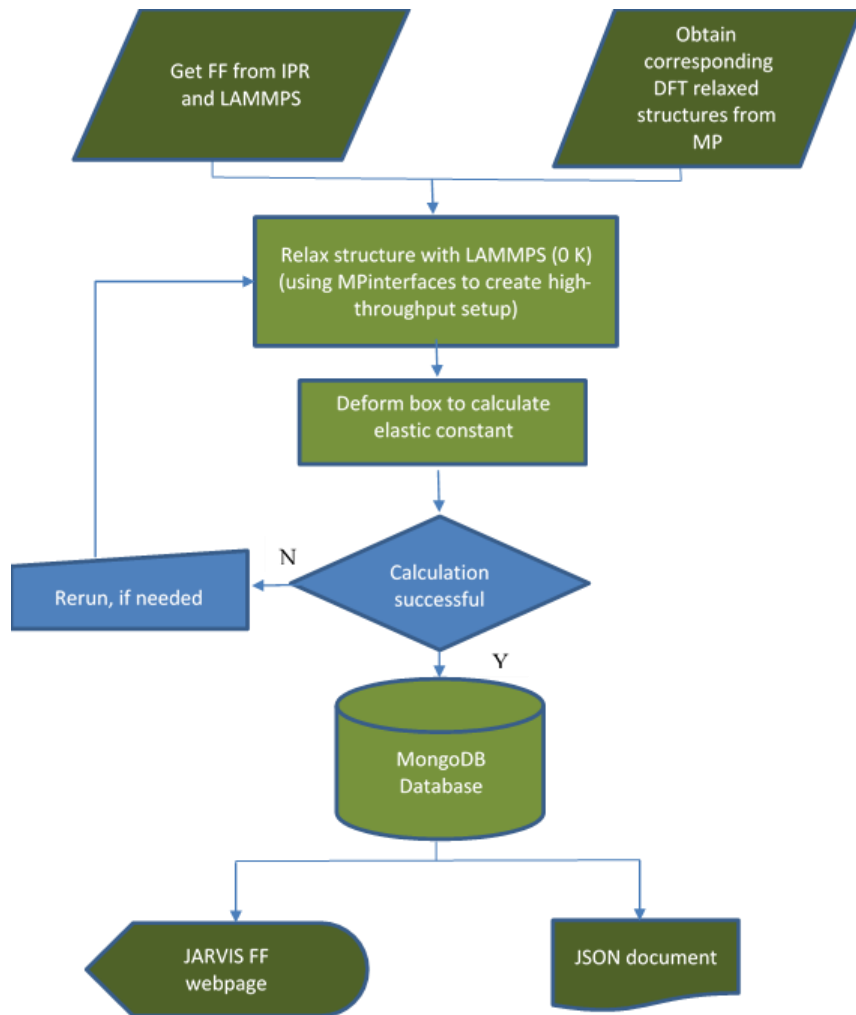
[Data Sites](#) - WWW sites with data useable as LAMMPS input or that archive LAMMPS output

- [JARVIS database for MD potential calculations on DFT geometries](#)
- [Cyberinfrastructure for Atomistic Materials Science \(CAMS\)](#)
- [Orsi group at Queen Mary University of London](#)

Outreach

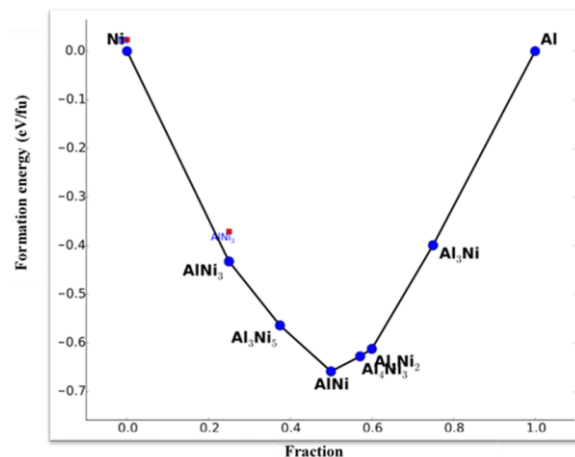
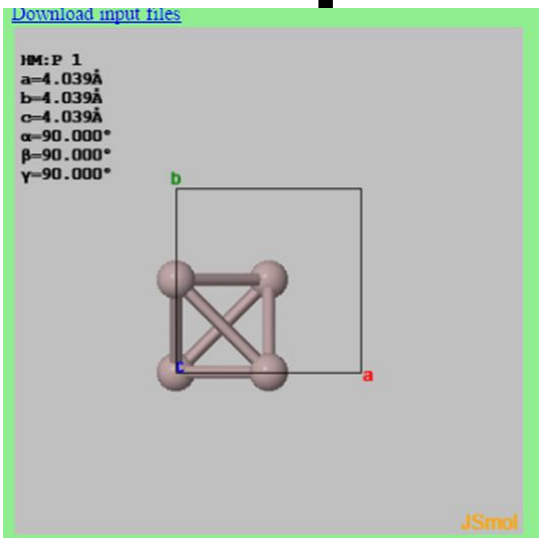
- ❖ Jarvis-FF has been recently added to the **"Pre/Post Processing Tools for use with LAMMPS"** (<http://lammps.sandia.gov/prepost.html#Jarvis>)

Technical details



- First we obtain the force-fields from interatomic potentials repository and LAMMPS potentials folder automatically, then corresponding DFT geometric structures are obtained from **Materials project** (**AFLOW** and **OQMD** databases will be integrated soon) with **REST-API**.
- JARVIS-FF **python scripts** creates all the necessary input files for LAMMPS calculation and creates a **MongoDB** after the calculation. All the stored data is provided on Github page in JSON file format.
- The interactive website is constructed with HTML5 and JavaScript. All the content of the website are provided at NIST-CTCMS website publicly <http://www.ctcms.nist.gov/~knc6/periodic.html>
- Entries with same formula but different force-fields are given same color to enhance visibility.
- The force-fields and input files for calculation are provided in **zipped format** to enhance data-reproducibility.

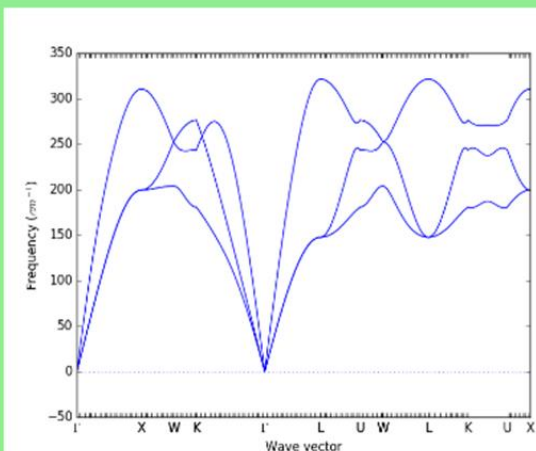
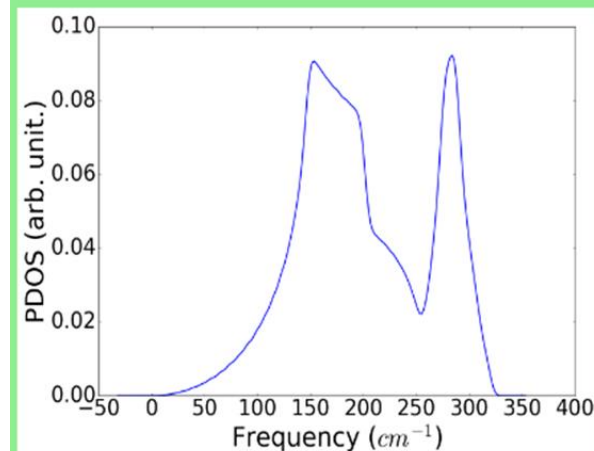
Examples of computed quantities



Convex-hull plot

Phonon

Phonons were obtained by making an interface of JARVIS-FF with [Phonopy package](#) at 0 K. For deformed-structures, constant volume ensemble was used. The deformed structures were taken of at least 1.5 nm size in all directions. The band-indices for phonon bandstructure was obtained with [Pymatgen](#). The phonon representation were obtained with phonopy. The code for their Infrared (I) or Raman (R) activity is not directly implemented in Phonopy. The I, R designations were implemented in JARVIS and will be released in public domain soon.



[Visualize Phonons here](#)

Phonon mode (cm^{-1}) Representation

-1.3684e-05 T1u I

All phonon mode at Gamma point (cm^{-1})

-1.3874e-05

-1.2885e-05

-1.03024e-05

199.579415818

310.632537509

Surface energy (J/m²)

Surface energies were calculated for symmetrically distinct crystal surfaces obtained with [Pymatgen](#). In the table, (hkl) indices and surface energies are given. For surface-structure energetics, constant volume ensemble was used. We impose the slab thickness to be at least 2 nm and vacuum size of 2.5 nm. The maximum miller index is taken as 3.

Surface Value

(1 1 1) 0.875

(1 0 0) 0.949

(3 3 2) 0.952

(3 2 2) 0.977

(2 1 1) 0.999

(3 3 1) 1.006

(1 1 0) 1.013

(3 1 1) 1.019

(3 2 1) 1.033

(3 1 0) 1.042

(3 2 0) 1.05

(2 1 0) 1.053

(2 2 1) 1.058

Vacancy-formation energy (eV)

Vacancy formation energies were calculated by deleting the symmetrically distinct atoms in the system. In the table, vacancy forming element, its multiplicity, and defect-formation energy are given. The reference element cohesive energies were calculated with the most stable structure for the element found on materials project database. The defect structures were generated with [Pydii](#) at 0 K. Defect structures were constructed with the fully-relaxed bulk system as input. For defect-structures energetics calculations, constant volume ensemble was used. We impose the defect structures to be at least 1.5 nm large in all directions.

Element Mult. Value

Al 4 0.674