

NIST Interatomic Potentials Repository Project

Lucas M. Hale





INTERATOMIC POTENTIALS REPOSITORY

https://www.ctcms.nist.gov/potentials/

260+ potentials

- Known provenance
- Any format
- Full citation and abstracts
- Property calculations

Incorporated into many projects

- OpenKIM
- JARVIS-FF
- pyiron
- MedeA

DOIs for hosted files in progress

el This site is currently being redesigned. Please let us know any feedback on the new design or if you find something incorrectinot working

Overview

Interatomic Potentials Repository

This repository provides a source for interatomic potentials (force fields), related files, and evaluation tools to help researchers obtain interatomic models and judge their quality and applicability. Users are encouraged to download and use interatomic potentials, with proper acknowledgement, and developers are welcome to contribute potentials for inclusion. The files provided have been submitted or vetted by their developers and appropriate references are provided. All classes of potentials (e.g., MEAM, ADP, COMB, Reax, EAM, etc.) and



materials are welcome. Interatomic potentials and/or related files are currently available for various metals, semiconductors, oxides, and carbon-containing systems.

Interatomic Potentials (Force fields)





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2006--Williams-P-L-Mishin-Y-Hamilton-J-C--Ag

Citation: P.L. Williams, Y. Mishin, and J.C. Hamilton (2006), "An embedded-atom potential for the Cu-Ag system", *Modelling and Simulation in Materials Science and Engineering*, **14(5)**, 817-833. DOI: 10.1088/0965-0393/14/5/002.

Abstract: A new embedded-atom method (EAM) potential has been constructed for Ag by fitting to experimental and first-principles data. The potential accurately reproduces the lattice parameter, cohesive energy, elastic constants, phonon frequencies, thermal expansion, lattice-defect energies, as well as energies of alternate structures of Ag. Combining this potential with an existing EAM potential for Cu, a binary potential set for the Cu–Ag system has been constructed by fitting the cross-interaction function to first-principles energies of imaginary Cu–Ag compounds. Although properties used in the fit refer to the 0 K temperature (except for thermal expansion factors of pure Cu and Ag) and do not include liquid configurations, the potentials demonstrate good transferability to high-temperature properties. In particular, the entire Cu–Ag phase diagram calculated with the new potentials in conjunction with Monte Carlo simulations is in satisfactory agreement with experiment. This agreement suggests that EAM potentials accurately fit to 0 K properties can be capable of correctly predicting simple phase diagrams. Possible applications of the new potential set are outlined.

EAM tabulated functions Notes: These files were provided by Yuri Mishin. File(s): Ag $F(\rho)$: F_ag.plt Ag $\rho(r)$: fag.plt Ag $\phi(r)$: pag.plt

LAMMPS pair_style eam/alloy (2006--Williams-P-L--Ag--LAMMPS--ipr1) See Computed Properties

Notes: This conversion was produced by Chandler Becker on 4 February 2009 from the plt files listed above. This version is compatible with LAMMPS. Validation and usage information can be found in Ag06_releaseNotes_1.pdf. If you use this setfl file, please credit the website in addition to the original reference. File(s): Ag.eam.alloy Ag06_releaseNotes_1.pdf



INTERATOMIC POTENTIALS REPOSITORY

Show computed properties for comparing potentials Full method descriptions + notes, disclaimers, version info

Select a composition: Ni Download data Click on plot to load interactive version



Cohesive Energy vs. Interatomic Spacing

Plots of the cohesive energy vs interatomic spacing, r, are shown below for a number of crystal structures. The values were computed using the iprPy E_vs_r_scan calculation method. The structures are generated based on the ideal atomic positions and b/a and c/a lattice parameter ratios for a given crystal prototype. The size of the system is then uniformly scaled, and the energy calculated without relaxing the system. To obtain these plots, values of r are evaluated every 0.02 Å up to 6 Å. Clicking on the image of a plot will open an interactive version of it in a new tab. The underlying data for the plots can be downloaded by clicking on the links above each plot.

Notes and Disclaimers

- These values are meant to be guidelines for comparing potentials, not the absolute values for any potential's properties. Values listed here may change if the calculation
 methods are updated due to improvements/corrections. Variations in the values may occur for variations in calculation methods, simulation software and implementations of
 the interatomic potentials.
- The minima identified by this calculation do not guarantee that the associated crystal structures will be stable since no relaxation is performed.
- NIST disclaimer

Version Information:

- 2019-02-04. Values regenerated with even r spacings of 0.02 Å, and now include values less than 2 Å when possible. Updated calculation method and parameters enhance compatibility with more potential styles.
- 2019-04-26. Results for hcp, double hcp, α-As and L1₀ prototypes regenerated from different unit cell representations. Only α-As results show noticable (>1e-5 eV) difference due to using a different coordinate for Wykoff site c position.
- 2018-06-13. Values for MEAM potentials corrected. Dynamic versions of the plots moved to separate pages to improve page loading. Cosmetic changes to how data is shown and updates to the documentation.
- 2017-01-11. Replaced png pictures with interactive Bokeh plots. Data regenerated with 200 values of r instead of 300.
- 2016-09-28. Plots for binary structures added. Data and plots for elemental structures regenerated. Data values match the values of the previous version. Data table
 formatting slightly changed to increase precision and ensure spaces between large values. Composition added to plot title and structure names made longer.
- 2016-04-07. Plots for elemental structures added.



NEW CALCULATIONS

Elastic Constants Predictions

Static elastic constants are displayed for the unique structures identified in Crystal Structure Predictions above. The values displayed here are obtained by measuring the change in virial stresses due to applying small strains to the relaxed crystals. The initial structure and the strained states are all relaxed using force minimization.

Notes and Disclaimers:

- These values are meant to be guidelines for comparing potentials, not the absolute values for any
 potential's properties. Values listed here may change if the calculation methods are updated due to
 improvements/corrections. Variations in the values may occur for variations in calculation methods,
 simulation software and implementations of the interatomic potentials.
- The presence of any structures in this list does not guarantee that those structures are stable.
- The elastic constants have been computed for a variety of strains, and in some cases for slightly
 different lattice constant values. The static nature of this calculation can give poor predictions if the
 evaluated states straddle a functional discontinuity in the potential's third derivative. Be sure to compare
 the elastic constants for the different strains (positive and negative).
- NIST disclaimer

Version Information:

· 2019-08-07. Data added.



Cij in GPa:

124.239	93.874	93.874	-0.0	-0.0	0.0
93.874	124.239	93.874	-0.0	-0.0	0.0
93.874	93.874	124.239	-0.0	-0.0	0.0
0.0	0.0	0.0	46.419	0.0	-0.0
0.0	0.0	0.0	-0.0	46.419	0.0
0.0	0.0	0.0	-0.0	-0.0	46.419

Diatom Energy vs. Interatomic Spacing

Plots of the potential energy vs interatomic spacing, r, are shown below for all diatom sets associated with the interatomic potential. This calculation provides insights into the functional form of the potential's two-body interactions. The values were computed using the iprPy diatom_scan calculation method. A system consisting of only two atoms is created, and the potential energy is evaluated for the atoms separated by 0.02 Å <= r <= 6.0 > Å in intervals of 0.02 Å. Two plots are shown: one for the "standard" interaction distance range, and one for small values of r. The small r plot is useful for determining if the potential is suitable for radiation studies.

Clicking on the image of a plot will open an interactive version of it in a new tab. The underlying data for the plots can be downloaded by clicking on the links above each plot.

Notes and Disclaimers:

- These values are meant to be guidelines for comparing potentials, not the absolute values for any potential's properties. Values listed here may change if the calculation
 methods are updated due to improvements/corrections. Variations in the values may occur for variations in calculation methods, simulation software and implementations of
 the interatomic potentials.
- · As this calculation only involves two atoms, it neglects any multi-body interactions that may be important in molecules, liquids and crystals.
- NIST disclaimer

Version Information:

· 2019-08-07. Plots added.

Download data

Click on plot to load interactive version

Click on plot to load interactive version

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NEW CALCULATIONS

Free Surface Formation Energy Predictions

Static free surface formation energies are displayed for select crystals. The values displayed here are obtained by taking a perfect periodic bulk crystal, slicing along a crystallographic plane, and using force minimization to statically relax the surfaces. The free surface formation energy is computed by comparing the energy of the defect system to the bulk system and dividing by the total surface area created by the cut.

Notes and Disclaimers:

- These values are meant to be guidelines for comparing potentials, not the absolute values for any
 potential's properties. Values listed here may change if the calculation methods are updated due to
 improvements/corrections. Variations in the values may occur for variations in calculation methods,
 simulation software and implementations of the interatomic potentials.
- The calculation only performs straight cuts along crystallographic planes and static relaxations. Lower
 energy configurations may exist that require atomic restructuring of the surfaces.
- Multiple values may be listed for a given plane followed by a number indicating different unique atomic
 planar cuts for the same theoretical plane. NOTE: currently, all #2 variations need to be redone as the
 plane positions were accidentally left the same as the #1 variations.
- NIST disclaimer

Version Information:

2019-08-07. Data added.

Composition: Ag ▼ Prototype: A1--Cu--fcc ▼ a₀: 4.090000144890601 ▼ Download raw data

Surface	Vfa (mJ/m²)
(331)	1002.7
(311)	1015.17
(110)	1016.82
(321)	1033.17
(310)	1046.67
(320)	1056.24
(210)	1061.75
(111)	862.21
(100)	940.43
(332)	942.78
(322)	950.37
(221)	976.61
(211)	990.88

Stacking Fault Energy Predictions

Stacking fault energy plots and maps are displayed for select crystals. The values are computed by

- 1. Starting with a bulk crystal system
- 2. Creating a free surface along one of the system's periodic boundaries and using force minimization to relax it
- 3. The system is sliced in half along a crystallographic plane parallel to the free surface. One half of the system is shifted relative to the other
- 4. The atoms in the shifted system are allowed to relax only in the direction normal to the shifting plane
- 5. The stacking fault energy for a given shift is computed by comparing the energy of the system before and after applying the shift, and dividing by the area of the fault plane

Notes and Disclaimers:

- These values are meant to be guidelines for comparing potentials, not the absolute values for any potential's properties. Values listed here may change if the calculation
 methods are updated due to improvements/corrections. Variations in the values may occur for variations in calculation methods, simulation software and implementations of
 the interatomic potentials.
- · Values between the measured points are interpolated and therefore may not perfectly capture minima and maxima.
- Multiple values may be listed for a given plane followed by a number indicating different unique atomic planar cuts for the same theoretical plane. NOTE: currently, all #2
 variations need to be redone as the plane positions were accidentally left the same as the #1 variations.
- NIST disclaimer

Version Information:

· 2019-08-07. Plots added.

Composition: Ag ▼ Prototype: A1--Cu--fcc ▼ a₀: 4.090000144890601 ▼ plot: (111) ▼ Download raw data



NEW CALCULATIONS

Free Surface Formation Energy Predictions

Static free surface formation energies are displayed for select crystals. The values displayed here are obtained by taking a perfect periodic bulk crystal, slicing along a crystallographic plane, and using force minimization to statically relax the surfaces. The free surface formation energy is computed by comparing the energy of the defect system to the bulk system and dividing by the total surface area created by the cut.

Notes and Disclaimers:

- These values are meant to be guidelines for comparing potentials, not the absolute values for any
 potential's properties. Values listed here may change if the calculation methods are updated due to
 improvements/corrections. Variations in the values may occur for variations in calculation methods,
 simulation software and implementations of the interatomic potentials.
- The calculation only performs straight cuts along crystallographic planes and static relaxations. Lower
 energy configurations may exist that require atomic restructuring of the surfaces.
- Multiple values may be listed for a given plane followed by a number indicating different unique atomic
 planar cuts for the same theoretical plane. NOTE: currently, all #2 variations need to be redone as the
 plane positions were accidentally left the same as the #1 variations.
- NIST disclaimer

Version Information:

2019-08-07. Data added.

Composition: Ag ▼ Prototype: A1--Cu--fcc ▼ a₀: 4.090000144890601 ▼ Download raw data

Surface	γ _{f≋} (mJ/m²)
(331)	1002.7
(311)	1015.17
(110)	1016.82
(321)	1033.17
(310)	1046.67
(320)	1056.24
(210)	1061.75
(111)	862.21
(100)	940.43
(332)	942.78
(322)	950.37
(221)	976.61
(211)	990.88

Stacking Fault Energy Predictions

Stacking fault energy plots and maps are displayed for select crystals. The values are computed by

- 1. Starting with a bulk crystal system
- 2. Creating a free surface along one of the system's periodic boundaries and using force minimization to relax it
- 3. The system is sliced in half along a crystallographic plane parallel to the free surface. One half of the system is shifted relative to the other
- 4. The atoms in the shifted system are allowed to relax only in the direction normal to the shifting plane
- 5. The stacking fault energy for a given shift is computed by comparing the energy of the system before and after applying the shift, and dividing by the area of the fault plane

Notes and Disclaimers:

- These values are meant to be guidelines for comparing potentials, not the absolute values for any potential's properties. Values listed here may change if the calculation
 methods are updated due to improvements/corrections. Variations in the values may occur for variations in calculation methods, simulation software and implementations of
 the interatomic potentials.
- · Values between the measured points are interpolated and therefore may not perfectly capture minima and maxima.
- Multiple values may be listed for a given plane followed by a number indicating different unique atomic planar cuts for the same theoretical plane. NOTE: currently, all #2
 variations need to be redone as the plane positions were accidentally left the same as the #1 variations.
- NIST disclaimer

Version Information:

2019-08-07. Plots added.

Composition: <u>Ag</u> ▼ Prototype: <u>A1--Cu--fcc</u> ▼ a₀: <u>4.090000144890601</u> ▼ plot: <u>(111)</u> [-1., 0.5, 0.5] ▼ Download raw data



NEW POTENTIALS DATABASE!

- https://github.com/usnistgov/potentials
- Add, edit, search, copy, share, don't share...
- Links to
- Early prototype, want feedback

Search for potentials

The Database.search_potentials() method currently allows for searches based on

- author (str, optional) Author string to search for. Note that the citation info must exactly contain this field, so multiple a
- year (str, optional) Publication year to search for.
- elements (list, optional) Element models to search for. If multiple elements are listed, the results will be inclusive, i.e. a
 elements will be included.

```
potentials = potdb.search_potentials(
    #year = '2007',
    author = 'Mendelev',
    elements = 'Fe',
)
```

```
# Show ids for all matching potentials
for potential in potentials:
    print(potential.id)
```

```
2003--Mendelev-M-I-Han-S-Srolovitz-D-J-et-al--Fe-2
2003--Mendelev-M-I-Han-S-Srolovitz-D-J-et-al--Fe-5
2004--Ackland-G-J-Mendelev-M-I-Srolovitz-D-J-et-al--Fe-P
2005--Mendelev-M-I-Srolovitz-D-J-Ackland-G-J-Han-S--Al-Fe
2007--Mendelev-M-I-Han-S-Son-W-et-al--V-Fe
```

Show all implementations for a given potential

] # Select a potential potential = potentials[0]

> # Display full HTML content for that potential display(HTML(potdb.full_html(potentials[0])))

2003--Mendelev-M-I-Han-S-Srolovitz-D-J-et-al--Fe-2

Citation: M.I. Mendelev, S. Han, D.J. Srolovitz, G.J. Ackland, D.Y. Sun and M. Asta (2003), "Development of new interatomic potential Abstract: Two procedures were developed to fit interatomic potentials of the embedded-atom method (EAM) form and applied to determodel liquid and the second procedure uses experimental liquid structure factor data. These additional types of information were incorrelation. The new potentials (provided herein) are, on average, in better agreement with the experimental or first-principles lattice para potentials.

Notes: This listing is for the reference's Fe #2 interaction parameters.

LAMMPS pair_style eam/fs (2003--Mendelev-M-I--Fe-2--LAMMPS--ipr1) superseded Notes: This file was provided by Mikhail Mendelev on Jun 10, 2007. Except for comments, this file is identical to "Fe_mm.eam.fs" in the Files:

Fe_2.eam.fs

e a LAMMPS pair_style eam (2003--Mendelev-M-I--Fe-2--LAMMPS--ipr2) retracted Notes: Update 09 Mar 2009: The file for Fe #2 (Feb 22, 2009) was sent as a replacement for the Jun 10, 2007 file above. It better tre eV/atom for bcc with a=2.855324 A. For archival purposes, the file can be found here. Thanks to Jianyang Wu for bringing this to our Files:

Fe_2.eam

LAMMPS pair_style eam/fs (2003--Mendelev-M-I--Fe-2--LAMMPS--ipr3) Notes: This file supports radial distances smaller than 0.5 A and gives the proper values of -4.1224351 eV/atom for a = 2.855324 A (I Files: Fe 2.eam.fs

OpenKIM (MO_769582363439) Notes: Taken from https://openkim.org. This KIM potential is based on the files from 2003--Mendelev-M-I--Fe-2--LAMMPS--ipr3. Links: EAM_Dynamo_MendelevHanSrolovitz_2003Potential2_Fe__MO_769582363439_005

OpenKIM (MO_856295952425) Notes: Taken from https://openkim.org. Links: EAM_MagneticCubic_MendelevHanSrolovitz_2003_Fe__MO_856295952425_002

OpenKIM (MO_546673549085) Notes: Taken from https://openkim.org. This KIM potential is based on the files from 2003--Mendelev-M-I--Fe-2--LAMMPS--ipr3. Links: EAM_Dynamo_Mendelev_2003_Fe__MO_546673549085_000

OpenKIM (MO_807997826449) superseded Notes: Taken from https://openkim.org. This KIM potential is based on the files from 2003--Mendelev-M-I--Fe-2--LAMMPS--ipr1. Links: EAM_Dynamo_MendelevHanSrolovitz_2003_Fe__MO_807997826449_000

ATOMMAN : ATOMISTIC MANIPULATION TOOLKIT

https://www.ctcms.nist.gov/potentials/atomman

pip install atomman

Generic atomic representation designed to support large-scale MD

- Focus on defect generation + analysis
- Potential and simulator agnostic
- Converters to/from ase, pymatgen, spglib, ... 25









High-throughput calculation methods

- source: https://github.com/usnistgov/iprPy
- docs: https://www.ctcms.nist.gov/potentials/iprPy

Make calculation methods as accessible as possible

- Openly available
- Low barrier for usage
- Transparent, documented methodologies
- Adaptable to new materials
- Transferable to other frameworks



Python script: pass parameter file to stand-alone script

Python class: call calculation methods directly

Jupyter Notebook: single document with documentation, code and example

High-throughput: prepare and execute with lists of parameter values

Input script for calc_E_vs_r_scan.px

Command lines for LAMMPS and MPI
lammps_command lmp_serial
mpi_command

Potential definition and directory containing associated files potential_file 1989--Adams-J-B--Ag--LAMMPS--ipr1.jgon potential_dir 1989--Adams-J-B--Ag--LAMMPS--ipr1

BORATORY

Initial system configuration to load load file A1--Cu--fcc.json load style system model load options family symbols Aα box parameters # System manipulations a uvw b uvw c uvw atomshift sizemults 5 5 5 # Units for input/output values length unit pressure unit energy unit force_unit # Run parameters minimum r 0.5 6 maximum r number of steps r 276 EASUREMEN



Python script: pass parameter file to stand-alone script

Python class: call calculation methods directly

Jupyter Notebook: single document with documentation, code and example

import atomman as am
import iprPy

```
cohesive_scan = iprPy.load_calculation('E_vs_r_scan')
```

```
lammps_command = 'lmp_mpi'
```

```
ucell = am.load('system_model', 'A1--Cu--fcc.json', symbols = 'Ag')
system = ucell.supersize(5, 5, 5)
```

potential = am.lammps.Potential('1989--Adams-J-B--Ag--LAMMPS--ipr1.json')

```
rmin = 0.5
rmax = 6
rsteps = 276
```

cohesive_scan.calc(lammps_command, system, potential, ucell, rmin, rmax, rsteps)

High-throughput: prepare and execute with lists of parameter values



Python script: pass parameter file to stand-alone script

Python class: call calculation methods directly

Jupyter Notebook: single document with documentation, code and example

High-throughput: prepare and execute with lists of parameter values



E_vs_r_scan Calculation

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Version: 2018-06-24

Disclaimers

Introduction

The E_vs_r_scan calculation calculation creates a plot of the cohesive energy vs interatomic spacing, r, for a given atomic system. The system size is uniformly scaled (b/a and c/a ratios held fixed) and the energy is calculated at a number of sizes without relaxing the system. All box sizes corresponding to energy minima are identified.

This calculation was created as a quick method for scanning the phase space of a crystal structure with a given potential in order to identify starting guesses for further structure refinement calculations.

Disclaimer #1: the minima identified by this calculation do not guarantee that the associated crystal structure will be stable as no relaxation is performed by this calculation. Upon relaxation, the atomic positions and box dimensions may transform the system to a different structure

Disclaimer #2: it is possible that the calculation may miss an existing minima for a crystal structure if it is outside the range of r values scanned, or has b/a, c/a values far from the ideal.

Method and Theory

An initial system (and corresponding unit cell system) is supplied. The r/a ratio is identified from the unit cell. The system is then uniformly scaled to all r_i values in the range to be explored and the energy for each is evaluated using LAMMPS and "run 0" command, i.e. no relaxations are performed.

In identifying energy minima along the curve, only the explored values are used without interpolation. In this way, the possible energy minima structures are identified for r_i where $E(r_i) < E(r_{i-1})$ and $E(r_i) < E(r_{i+1})$.

Demonstration



MATERIAL MEASUREMENT LABORATORY

STACKING FAULT GENERATION AND PLOTTING

Method relatively simple

- 2 directions periodic, one not (free surface)
- Shift half of system by in-plane vectors a_1, a_2
- Measure $E(a_1, a_2)$

Tricky for general system

- Fault planes given as Miller crystallographic (hkl) planes and [uvw] vectors relative to conventional unit cells
- $[hkl] \perp (hkl)$ only guaranteed for cubic systems
- System box vectors rotated from unit cell box vectors
- System box vectors a, b, c not aligned with x, y, z
- a_1, a_2 may or may not be aligned with a, b







STACKING FAULT GENERATION AND PLOTTING



Initialize the StackingFault object and check parameters

[11]: sf = am.defect.StackingFault(system, alvect=alvect, a2vect=a2vect, ucellbox=ucell.box, transform=tra

print('Fault system has', sf.system.natoms, 'total atoms.')
print('Fault system has', len(sf.system.atoms.atype[sf.abovefault]), 'atoms above the fault')
print('Fault plane is at z =', sf.faultposcart)
print()
print("Fault system's pbc is", sf.system.pbc)
print()
print('alvect as given:', sf.alvect)
print('Cartesian alvect:', sf.alvectcart)
print('avect as given:', sf.a2vect)
print('Cartesian a2vect:', sf.a2vectcart)

Fault system has 48 total atoms. Fault system has 24 atoms above the fault Fault plane is at z = 14.029611541307906

Fault system's pbc is [True True False]

alvect as given: [-0.5 0.5 0.] Cartesian alvect: [2.86378246e+00 -2.75990494e-16 -4.17652603e-16]

```
a2vect as given: [-0.5 0. 0.5]
Cartesian a2vect: [ 1.43189123e+00 2.48010836e+00 -4.17652603e-16]
```

Now, StackingFault.iterfaultmap() can generate a 2D map. Note that the <112> path corresponds to the points where a1 = a

```
[12]: for a1, a2, faultsystem in sf.iterfaultmap(num_a1=5, num_a2=5):
    d = am.displacement(system, faultsystem)[-1]
    print('a1 = %.1f, a2 = %.1f, d = [%7.4f %7.4f %7.4f]' % (a1, a2, d[0], d[1], d[2]))
    a1 = 0.0, a2 = 0.0, d = [ 0.0000 0.0000 0.0000]
    a1 = 0.2, a2 = 0.0, d = [ 0.5728 0.0000 0.0000]
```

al = 0.2, a2 = 0.0, d = [0.5728 0.0000 0.0000] al = 0.4, a2 = 0.0, d = [1.1455 0.0000 0.0000] al = 0.6, a2 = 0.0, d = [1.7183 -0.0000 0.0000] al = 0.8, a2 = 0.0, d = [2.2910 -0.0000 0.0000]



HIGH-THROUGHPUT GAMMA SURFACES

iprPy

- Unit cells for all fcc/bcc/hcp crystals + potentials selected
- Calculation script generates configurations + runs LAMMPS for each
- Results placed in JSON/XML database

DFT

- 1. Script generates configurations from unit cell
- 2. Each shift submitted separately
- 3. Results collected with another
- script into JSON format

Finished 2700+ 30x30 grids

atomman.defect.GammaSurface

Collects stacking fault energies and has methods for interpolations and plots

Finished 3 20x20 grids

NIST

atomman.defect.StackingFault

Generates stacking fault atomic

configurations for any crystal

and fault plane



Vacancy-formation energy (eV)

Vacancy formation energies were calculated by deleting the symmetrically distinct atoms in the The reference element cohesive energies were calculated with the most stable structure for the system as input. For defect-structures energetics calculations, constant volume ensemble was us

Element Mult. Value

Al 4 0.674 <u>Download cif file</u>

Surface energy (J/m²)

Surface energies were calculated for symmetrically distinct of impose the slab thickness to be at least 2 nm and vaccum siz

Nature: Scientific Data 4, 160125 (2017) J. Phys. Cond. Matt. 30, 395901(2018).

- Comparing classical and quantum data
 - Selecting appropriate potentials/FFs
 - Reliability of FFs
- Easy web-based search
- Automating atomistic calculations (all scripts on github)
- ~50000 LAMMPS calculations, ~1500 materials
- Machine learning

https://jarvis.nist.gov/

JARVIS 🗘 FF



Coming soon:

- Grain-boundary energies,
- Stacking faults,
- Machine learning FFs



Links to other databases or papers are provided below

JVASP-816

<u>mp-134</u>

Energy above hull from mp (eV): 0.0



MATERIALS RESOURCE REGISTRY

https://materials.registry.nist.gov/

- "Yellow pages" for materials tools Search current entries
- Add your own projects and data

NIST		Home	Services »	Login	Help	Contact
Ма	aterials Resou		gistry			
	ARCH FOR RESOURCES	ADD YOUR RES	OURCE			
Find Materials Data			Home	Page		
This system allows for the registration of materials re resources and the end users. The Materials Resource making the registered information available for rese	esources, bridging the gap betwee a Registry functions as a centrally l arch to the materials community.	en existing ocated service,	Service	s rch for resources		

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arch criteria used (Clear all):		261 result			
the v	See detailed metadata				
▲ TYPE (Clear)	Polymer Property Predictor and Database University of Chicago Visit resource's home po	qe			
 Corganization (51) Collection (26) Dataset (33) Consect (4) 	http://ppdb.uchicago.edu/ The Polymer Property Predictor and Database includes both a database of polymer interaction parameters (x transition temperatures, as well as tools to predict polymer properties and phase diagrams. Phase diagrams for neutral polymers (Flory- Huggins and Lattice Cluster Theory) and charged polymers (Voorn-Overbeek) of generated give show more), glass or both can be			
 Software (127) Web Site (22) 	ZENO Jack Douglas - NIST https://github.com/usnistgov/zeno Subject keyword(s): Monte Carlo, Stokes friction coefficient, Electrostatic capacity, Intrinsic viscosity, Intrinsic conduct	ivity,			
ORIGIN OF DATA (Clear) MATERIAL TYPE (Clear)	Electrical polarizability Efficient method for characterizing object shape and for calculating transport properties of nanoparticle synthetic and biological macromolecules. National Institute for Computational Sciences, Oak Ridge National Laboratory	es and			
▲ STRUCTURAL (Clear) FEATURE	University of Tennessee https://www.nics.tennessee.edu Subject keyword(s): high performance computing, large-scale data analysis, data visualization, XSEDE The National Institute for Computing Sciences (NICC) at the University of Tennessee Know illo is one of the leading				
 Composites (15) defects (13) 	high performance computing centers for excellence in the United States. NICS strives to accomplish [its] miss facilitating transformational scientific discovery by providing scientists and researchers from around show mo	sion by pre			
engineered structures (2)	Potfit Peter Brommer, Franz Gähler - Potfit				



ATOMISTIC SIMULATIONS FOR INDUSTRIAL NEEDS

2-3 day workshop in Rockville, MD in August, 2020

Talks and discussions fostering interactions between

- Potentials developers
- Tool developers
- Academic and industrial collegues
- Machine learning and data analysis experts

Now calling for co-organizers



LINKS

https://www.ctcms.nist.gov/potentials/ https://www.ctcms.nist.gov/potentials/atomman https://www.ctcms.nist.gov/potentials/iprPy

https://materials.registry.nist.gov/ https://jarvis.nist.gov/

https://github.com/usnistgov/potentials https://github.com/usnistgov/atomman https://github.com/usnistgov/iprPy NIST Interatomic Potentials Repository atomman documentation iprPy documentation

NIST Materials Resource Registry JARVIS

NIST Interatomic Potentials Database atomman source code iprPy source code

potentials@nist.gov

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