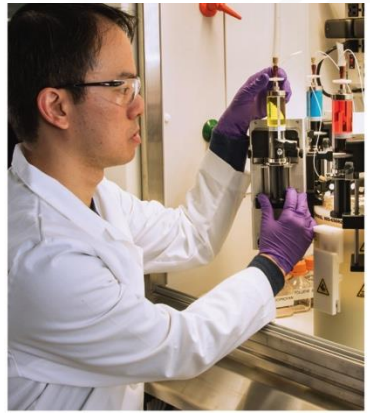
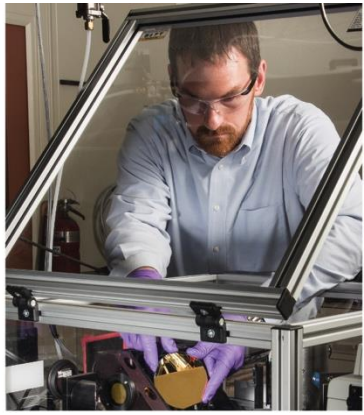




NIST Interatomic Potentials Repository Project

Lucas M. Hale

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

IPR

MATERIAL
MEASUREMENT
LABORATORY

INTERATOMIC POTENTIALS REPOSITORY

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

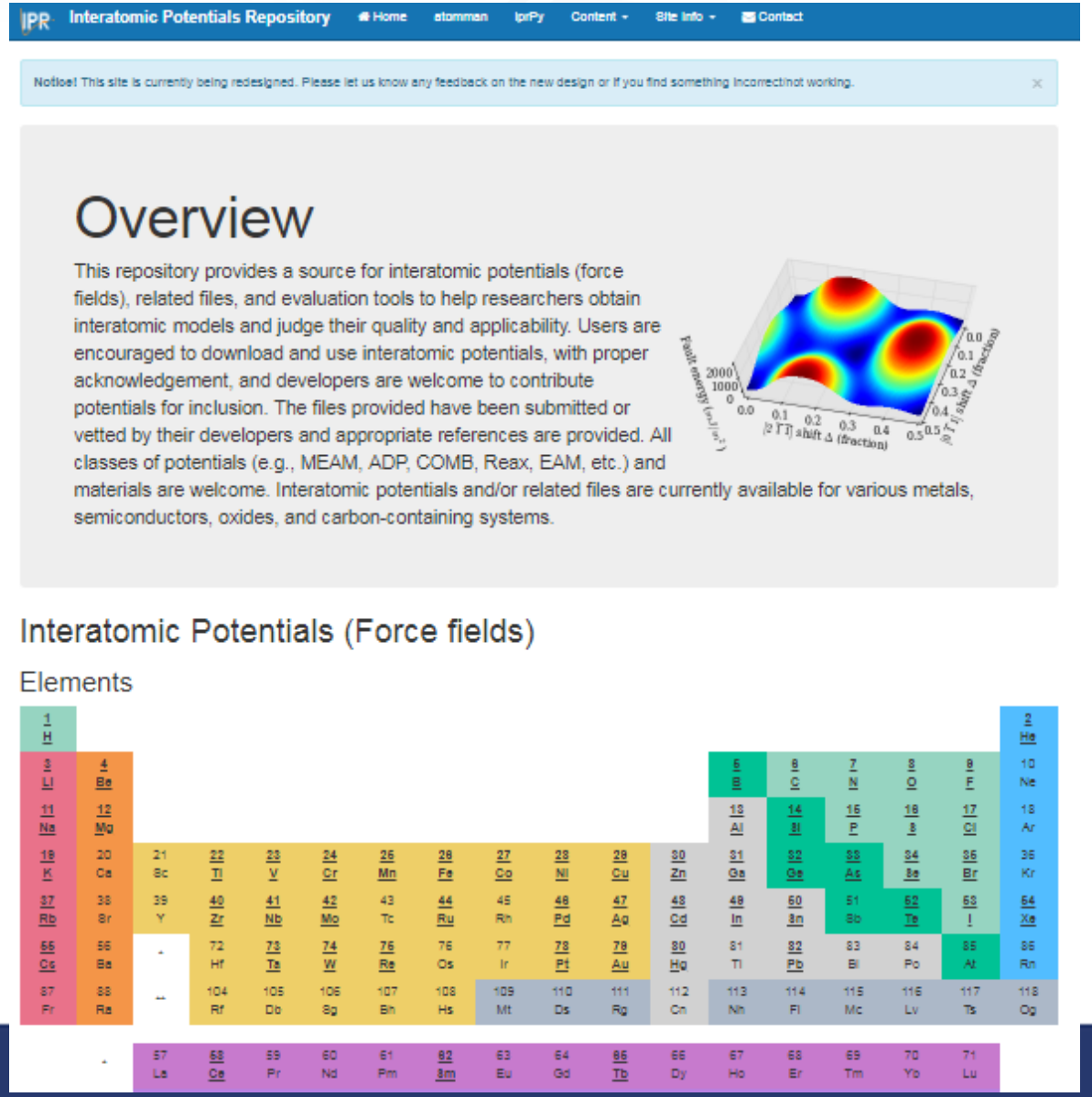
260+ potentials

- 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



INTERATOMIC POTENTIALS REPOSITORY

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260+ potentials

- Known provenance
- Any format
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Incorporated into many projects

- OpenKIM
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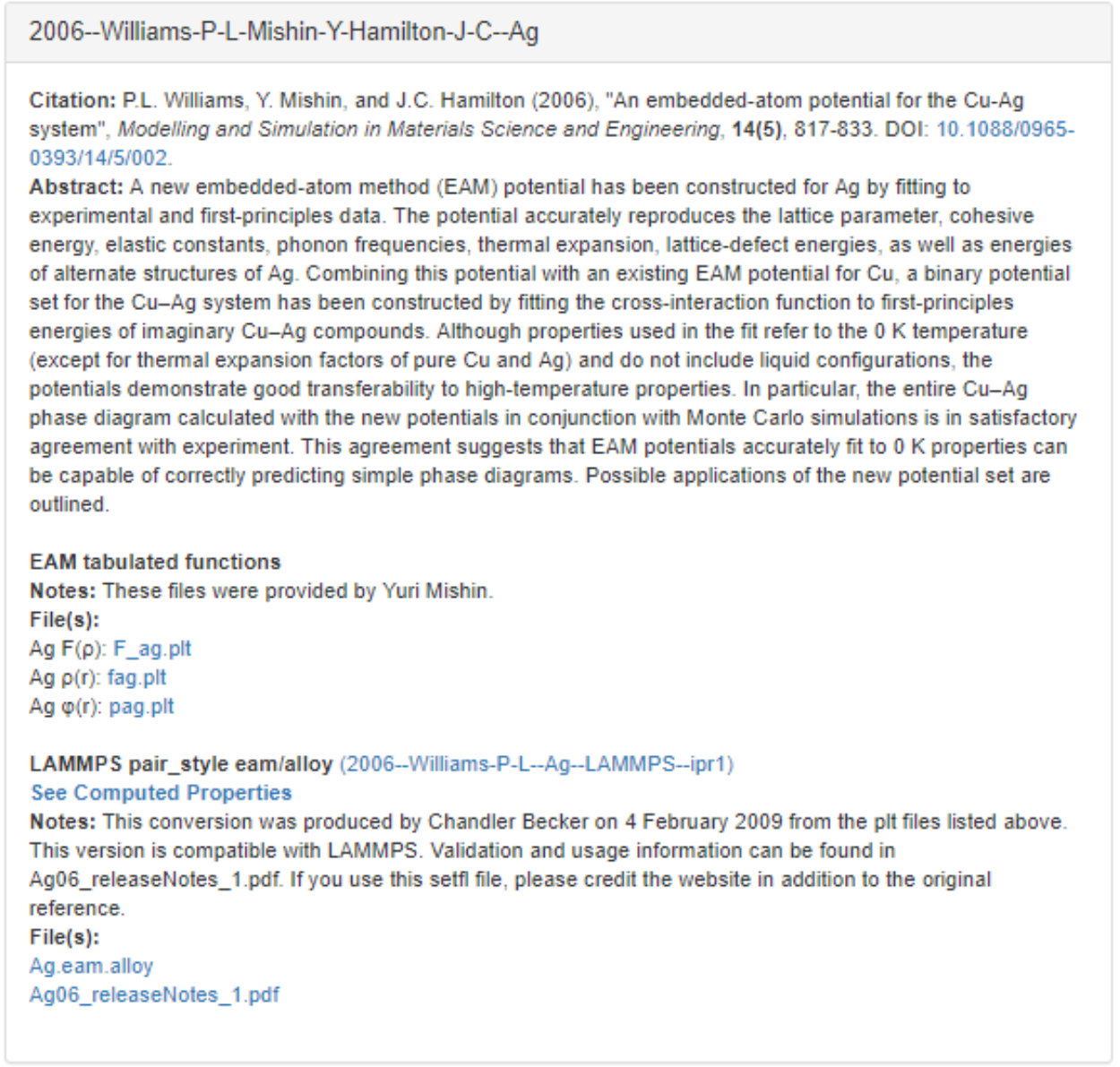
DOIs for hosted files in progress



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(ρ): F_ag.plt
Ag ρ(r): fag.plt
Ag φ(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

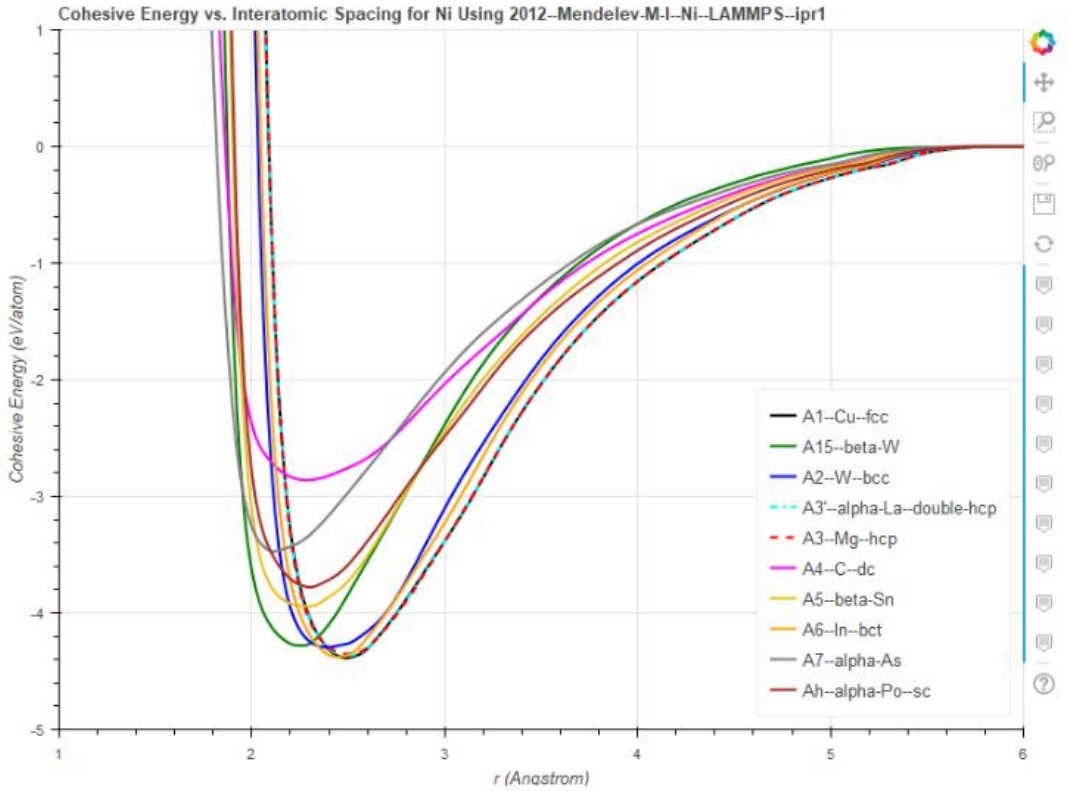
Full method descriptions + notes, disclaimers, version info

Interactive plots and downloadable raw data

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 $L1_0$ 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.

Composition: Ag ▼
Prototype: A1--Cu--fcc ▼
a_0: 4.090000144890601 ▼
strain: -1e-08 ▼
Download raw data

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:

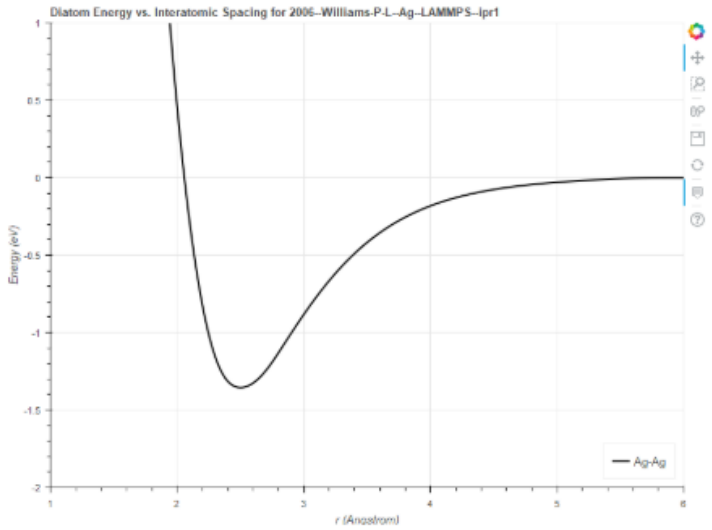
- These values are meant to be guidelines for comparing potentials, not the absolute values for any potential's properties. Values listed here may change if the calculation methods are updated due to improvements/corrections. Variations in the values may occur for variations in calculation methods, simulation 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:

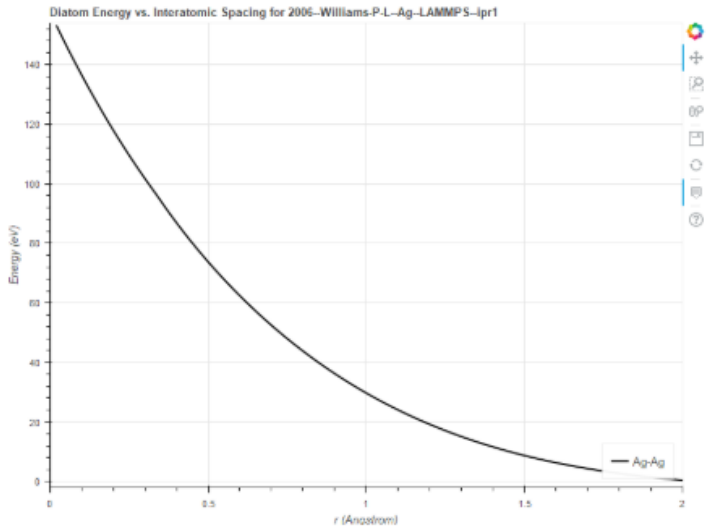
- 2019-08-07. Plots added.

Download data

Click on plot to load interactive version



Click on plot to load interactive version



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 ▼
a_0: 4.090000144890601 ▼
Download raw data

Surface	γ_{fs} (mJ/m^2)
(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

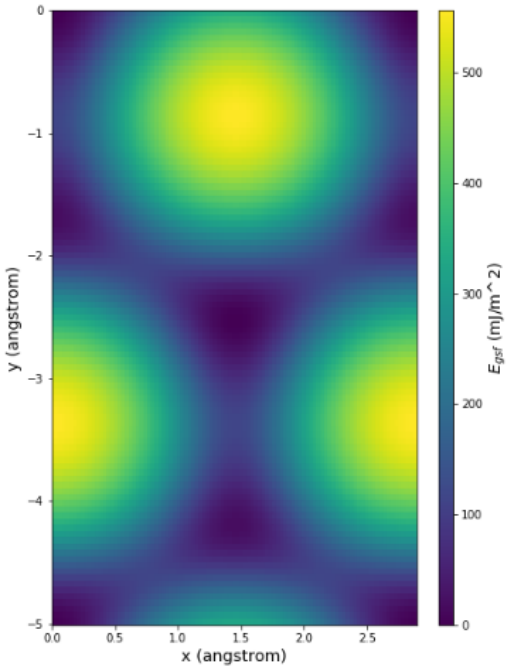
Notes and Disclaimers:

- 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 ▼
a_0: 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 ▼
a_0: 4.090000144890601 ▼
Download raw data

Surface	γ_{fs} (mJ/m^2)
(331)	1002.7
(311)	1015.17
(110)	1016.82
(321)	1033.17
(310)	1046.67
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(111)	862.21
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Stacking Fault Energy Predictions

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

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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

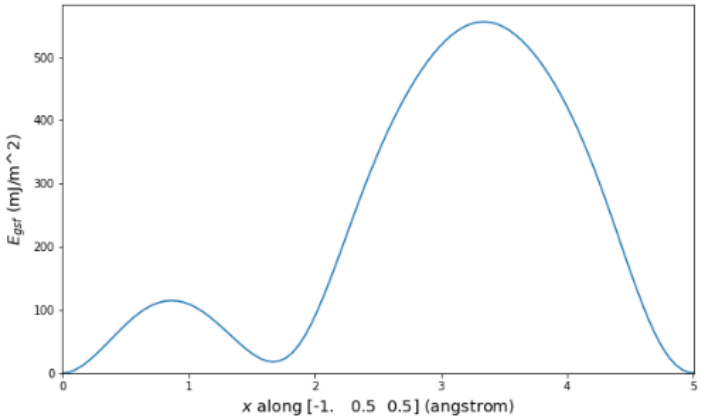
Notes and Disclaimers:

- 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 ▼
a_0: 4.090000144890601 ▼
plot: (111) [-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 potentia
Abstract: Two procedures were developed to fit interatomic potentials of the embedded-atom method (EAM) form and applied to dete model liquid and the second procedure uses experimental liquid structure factor data. These additional types of information were inco relation. 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 t
Files:
Fe_2.eam.fs

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 trea 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 (
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

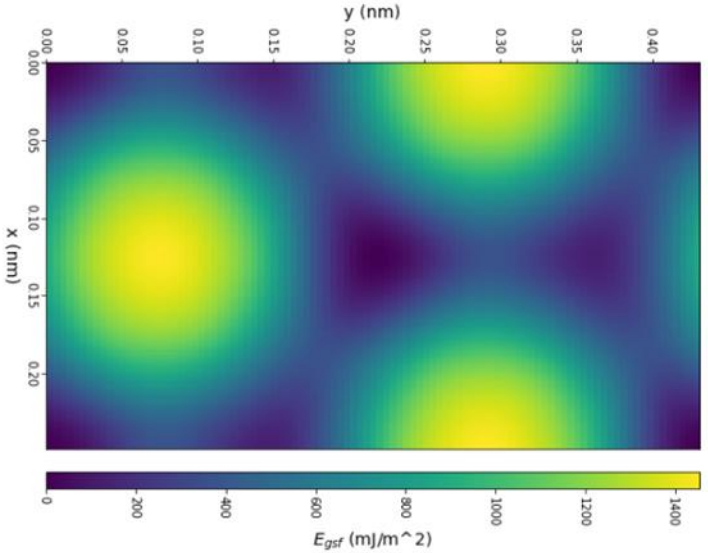
ATOMMAN : ATOMISTIC MANIPULATION TOOLKIT

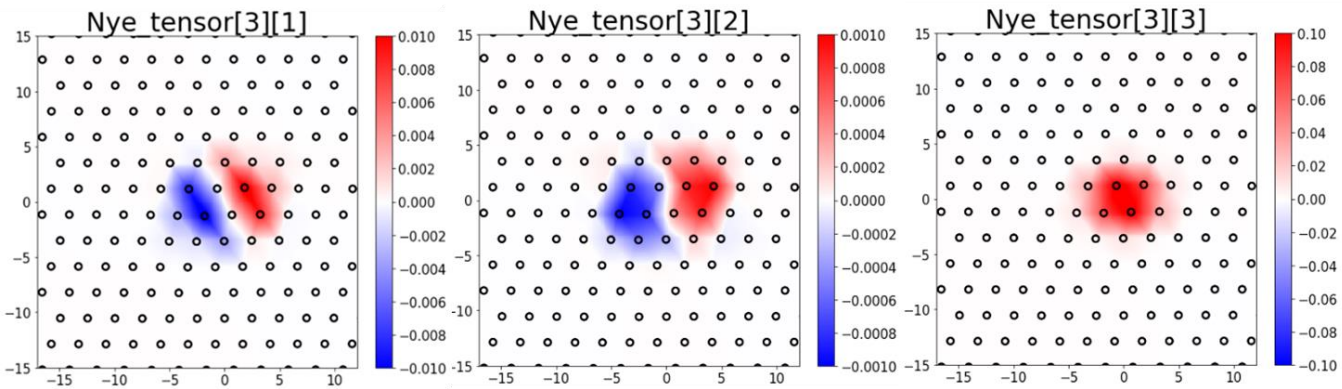
https://www.ctcms.nist.gov/potentials/atomman

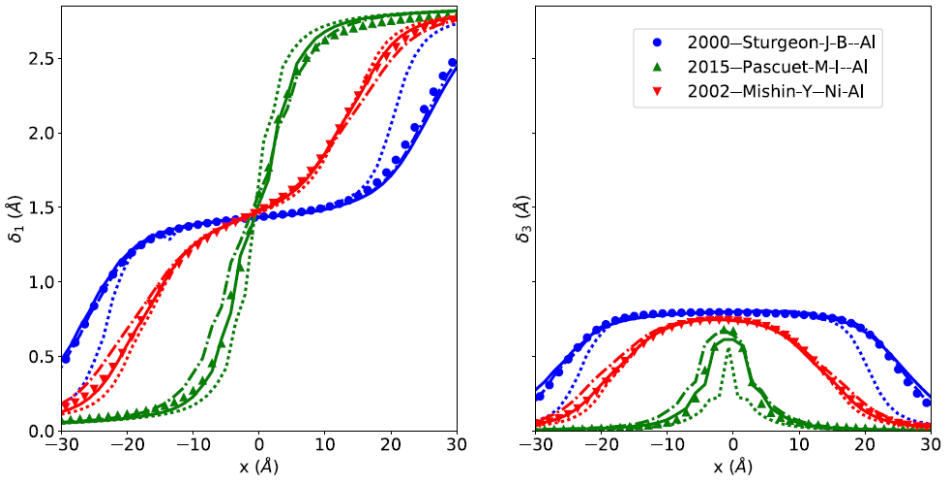
```
pip install atomman
```

Generic atomic representation designed to support large-scale MD

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







IPRPY CALCULATION FRAMEWORK

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

IPRPY CALCULATION FRAMEWORK

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.py

# 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.json
potential_dir               1989--Adams-J-B--Ag--LAMMPS--ipr1

# Initial system configuration to load
load_file                   A1--Cu--fcc.json
load_style                  system_model
load_options
family
symbols                     Ag
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
maximum_r                   6
number_of_steps_r           276
```

IPRPY CALCULATION FRAMEWORK

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

```
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)
```

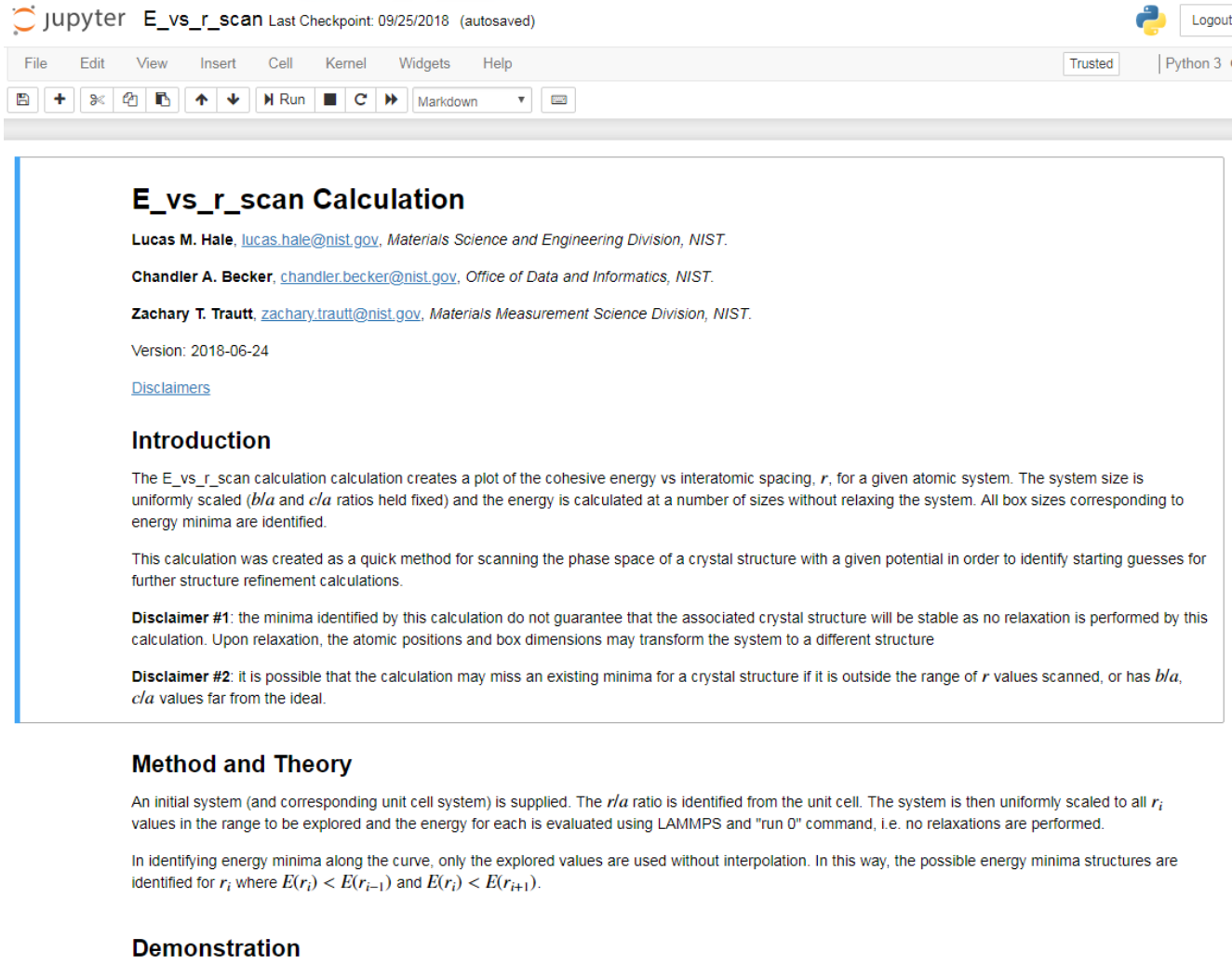
IPRPY CALCULATION FRAMEWORK

Python script: pass parameter file to stand-alone script

Python class: call calculation methods directly

Jupyter Notebook: single document with documentation, code and example

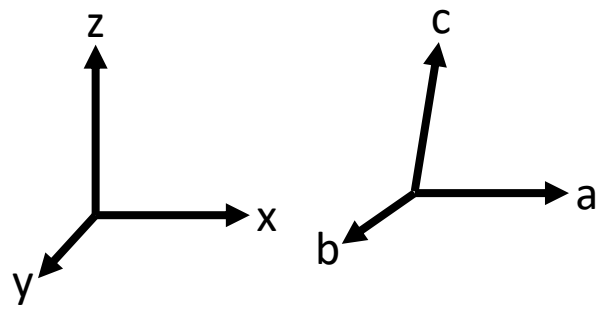
High-throughput: prepare and execute with lists of parameter values



STACKING FAULT GENERATION AND PLOTTING

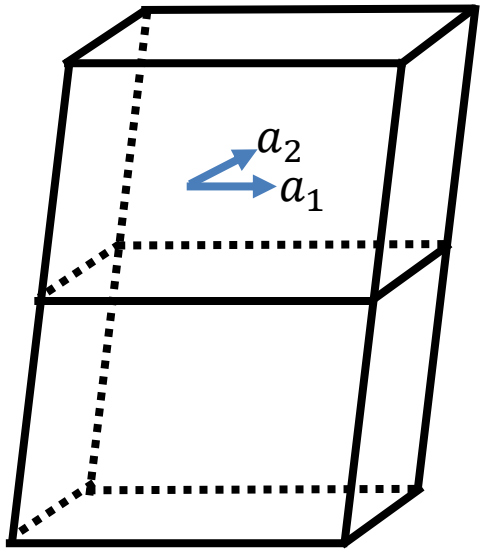
Method relatively simple

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



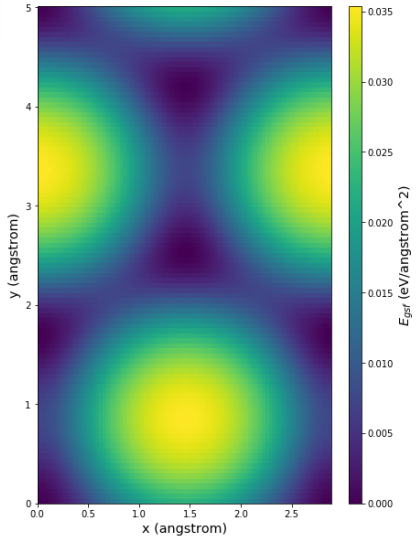
Tricky for general system

- Fault planes given as Miller crystallographic (hkl) planes and [uvw] vectors relative to conventional unit cells
- [hkl]⊥(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

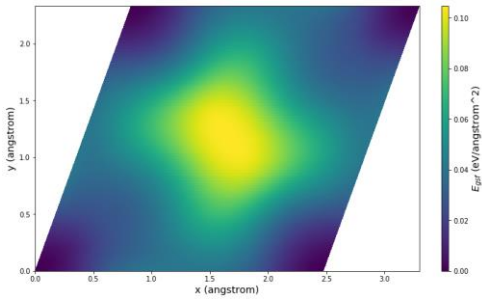


STACKING FAULT GENERATION AND PLOTTING

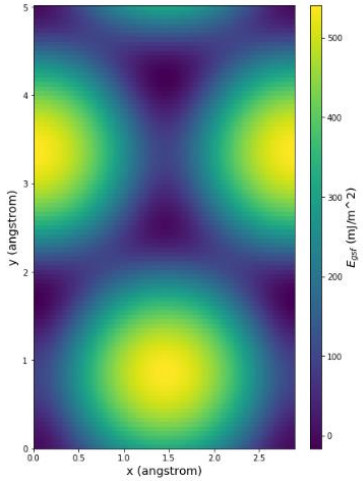
FCC (111)



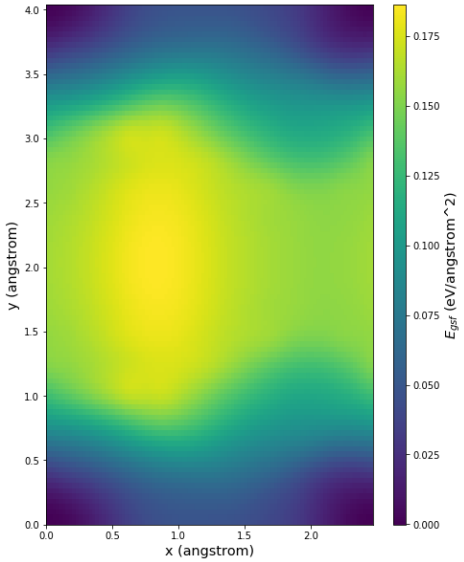
BCC (110)



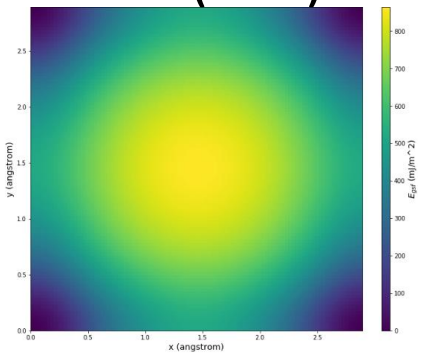
HCP (0001)



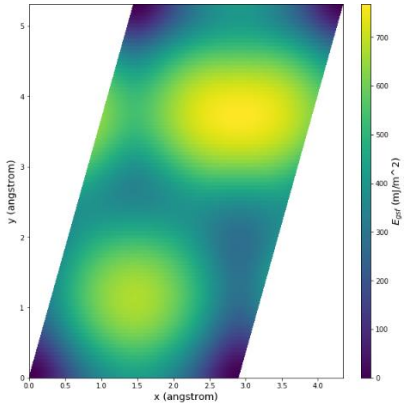
BCC (112)



FCC (100)



HCP (1011)



Initialize the StackingFault object and check parameters

[11]:
```
sf = am.defect.StackingFault(system, a1vect=a1vect, 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('a1vect as given:', sf.a1vect)
print('Cartesian a1vect:', sf.a1vectcart)
print()
print('a2vect as given:', sf.a2vect)
print('Cartesian a2vect:', sf.a2vectcart)
```

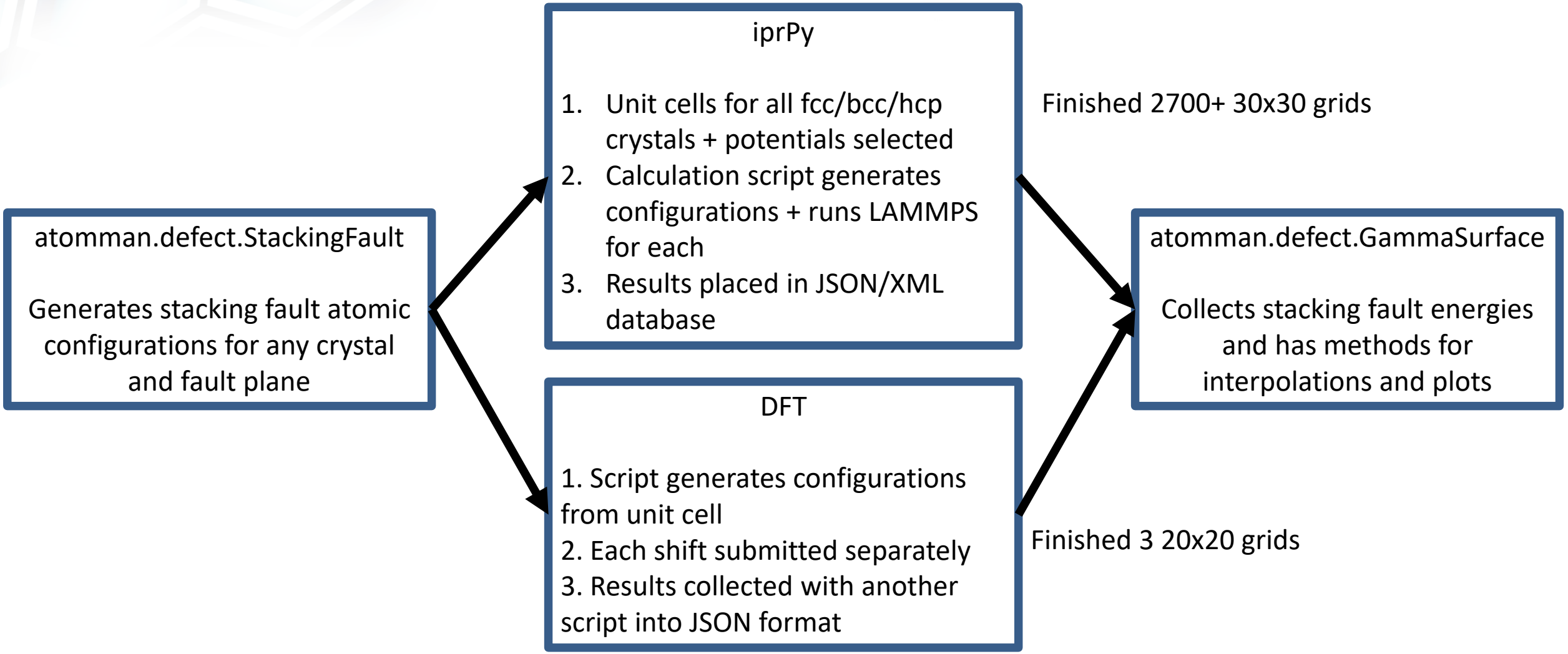
```
Fault system has 48 total atoms.
Fault system has 24 atoms above the fault
Fault plane is at z = 14.029611541307906

Fault system's pbc is [ True  True False]

a1vect as given: [-0.5  0.5  0. ]
Cartesian a1vect: [ 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 <$\bar{1}\bar{1}2$> path corresponds to the points where a1 = a2

[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]))
```

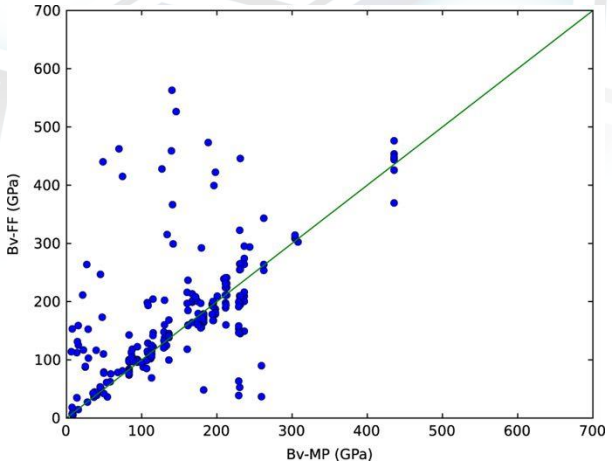
```
a1 = 0.0, a2 = 0.0, d = [ 0.0000  0.0000  0.0000]
a1 = 0.2, a2 = 0.0, d = [ 0.5728  0.0000  0.0000]
a1 = 0.4, a2 = 0.0, d = [ 1.1455  0.0000  0.0000]
a1 = 0.6, a2 = 0.0, d = [ 1.7183 -0.0000  0.0000]
a1 = 0.8, a2 = 0.0, d = [ 2.2910 -0.0000  0.0000]
```

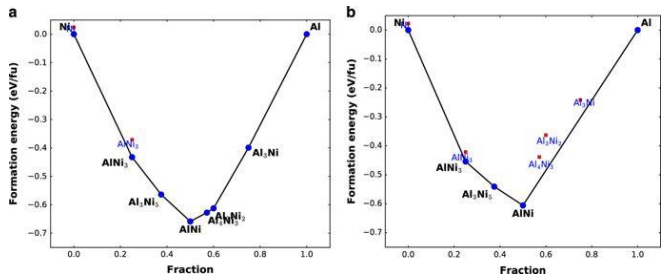
HIGH-THROUGHPUT GAMMA SURFACES



JARVIS-FF

- 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





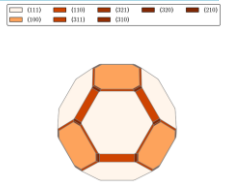
Vacancy-formation energy (eV)

Vacancy formation energies were calculated by deleting the symmterically 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 u

Element	Mult.	Value
Al	4	0.674 Download cif file

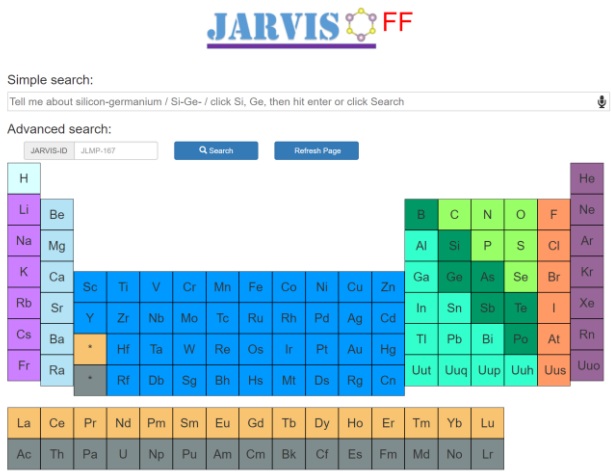
Surface energy (J/m^2)

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



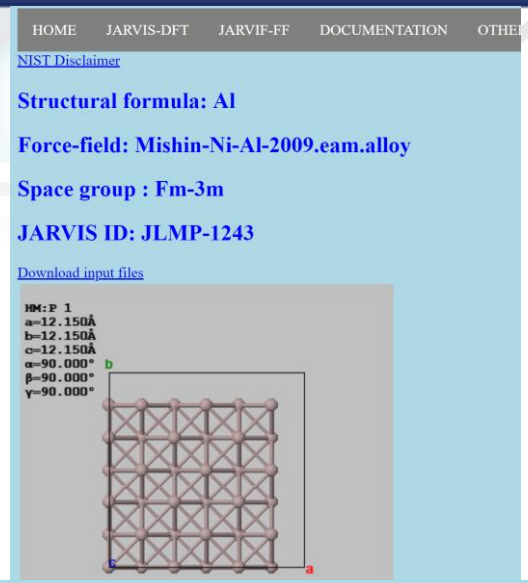
[Nature: Scientific Data 4, 160125 (2017)](#)
[J. Phys. Cond. Matt. 30, 395901(2018).](#)

https://jarvis.nist.gov/



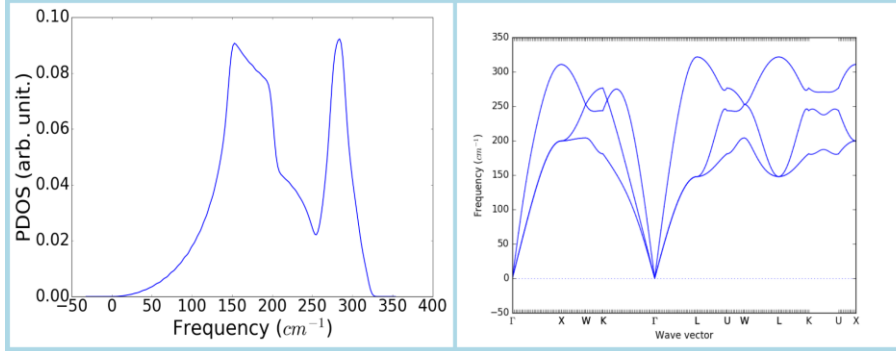
Coming soon:

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



Phonon

Phonons were obtained by making an interface of JARVIS-FF with Phonopy package at 0 K [Source] . For deformed-structures, constant volume e
least 1.5 nm size in all directions. The band-indices for phonon bandstructure was obtained with Pymatgen. The phonon representation were obtain
active modes respectively



See also

Links to other databases or papers are provided below

[JVASP-816](#)

[mp-134](#)

Energy above hull from mp (eV): 0.0

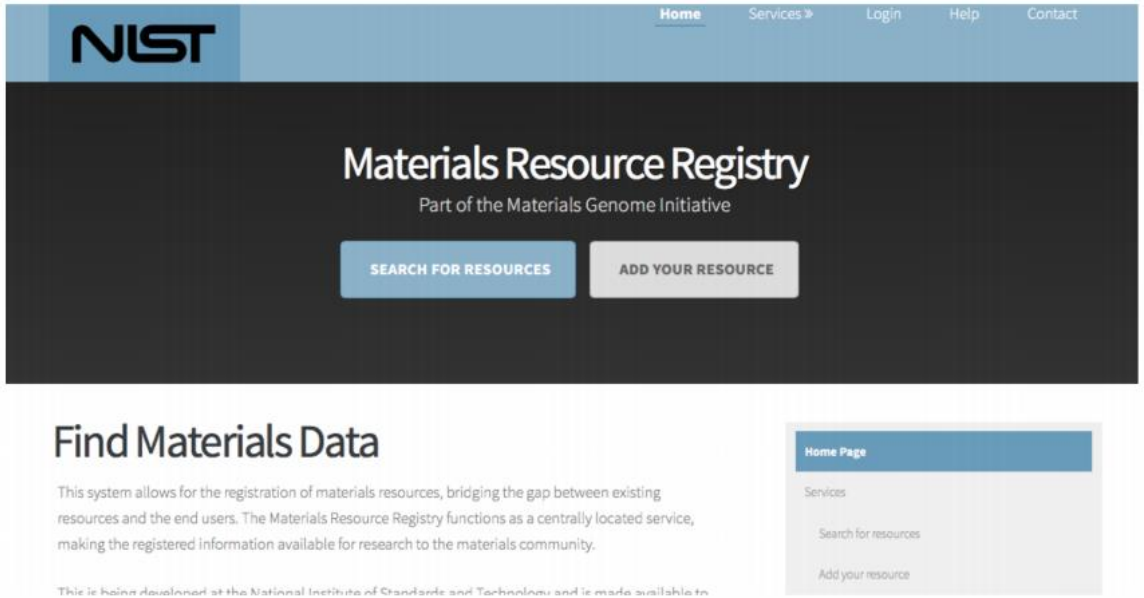
MATERIALS RESOURCE REGISTRY

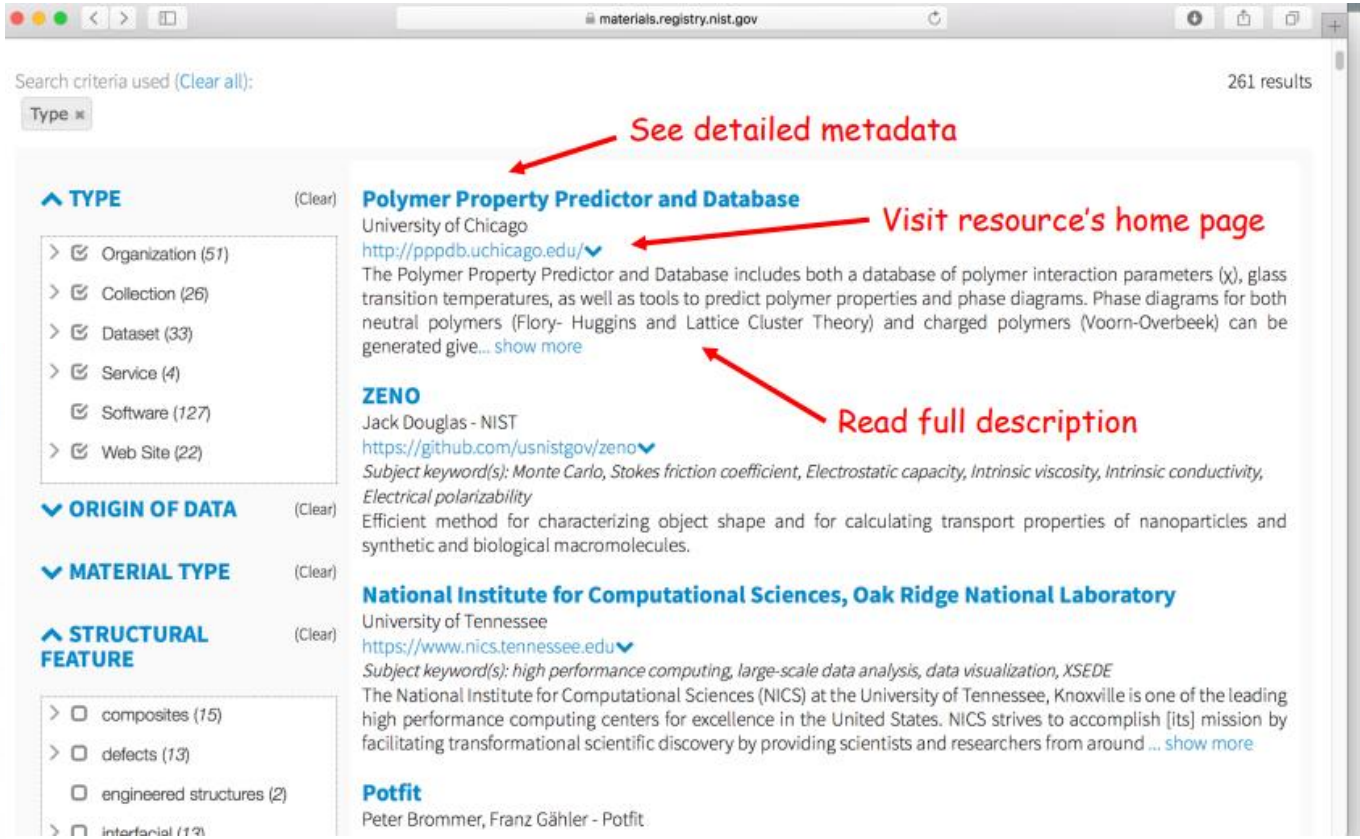
https://materials.registry.nist.gov/

"Yellow pages" for materials tools

Search current entries

Add your own projects and data





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	NIST Interatomic Potentials Repository
https://www.ctcms.nist.gov/potentials/atomman	atomman documentation
https://www.ctcms.nist.gov/potentials/iprPy	iprPy documentation
https://materials.registry.nist.gov/	NIST Materials Resource Registry
https://jarvis.nist.gov/	JARVIS
https://github.com/usnistgov/potentials	NIST Interatomic Potentials Database
https://github.com/usnistgov/atomman	atomman source code
https://github.com/usnistgov/iprPy	iprPy source code
potentials@nist.gov	Contact us