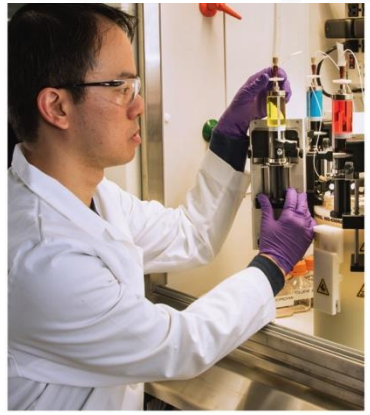
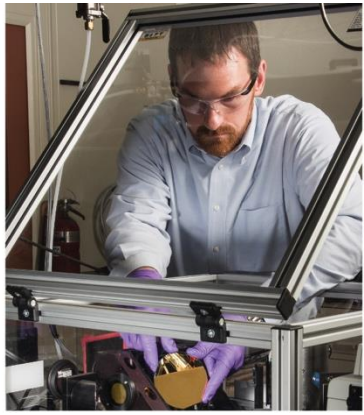




# Interatomic Potentials Repository Project

Lucas M. Hale
Zachary T. Trautt
Chandler A. Becker

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

IPR

MATERIAL MEASUREMENT LABORATORY

# MAJOR COMPONENTS OF IPR

NIST Interatomic Potentials Repository [1]

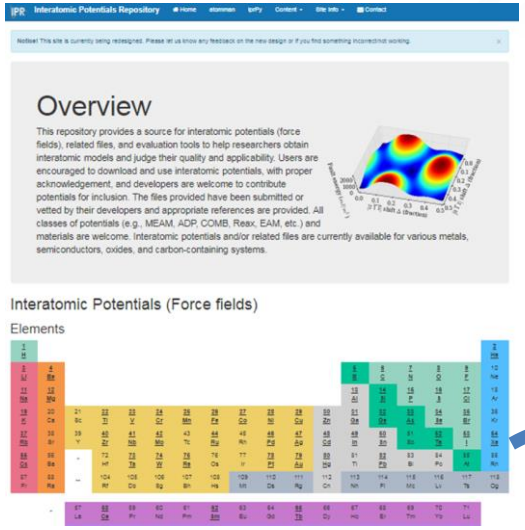
- Hosts +290 different interatomic potentials
- Computed properties for comparison

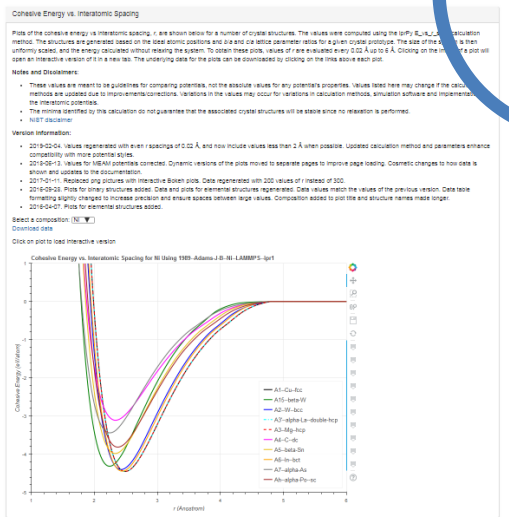
atomman Python package [2]

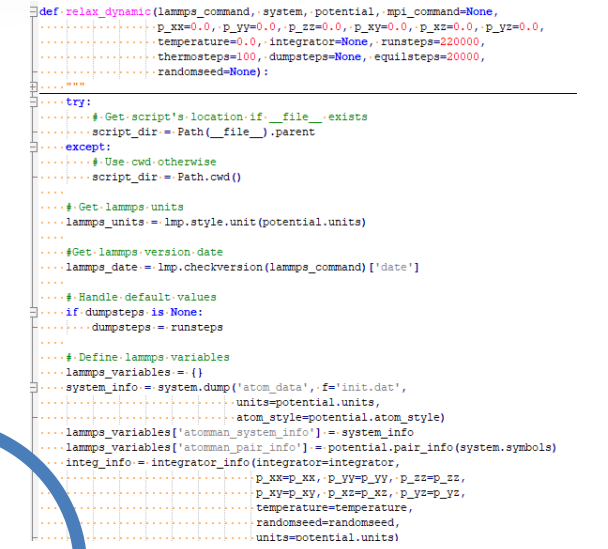
- Create and manipulate atomic configurations
- Interact with LAMMPS MD software [3]
- Focus on crystalline defects

iprPy Python package [2]

- Complete property calculations
- High-throughput workflow tools



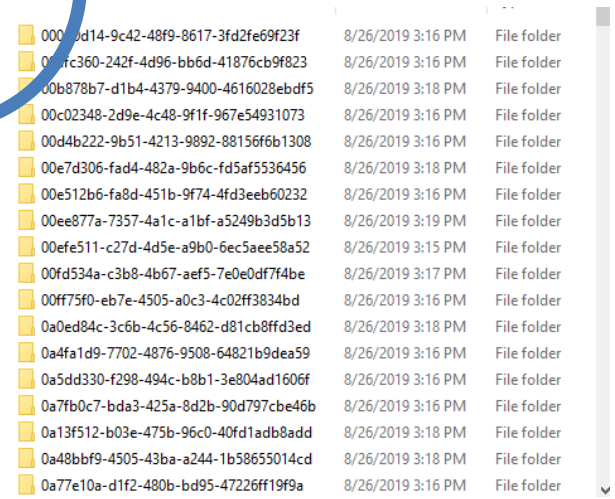
```
def relax_dynamic(lammps_command, system, potential, mpi_command=None,
                  p_xx=0.0, p_yy=0.0, p_zz=0.0, p_xy=0.0, p_xz=0.0, p_yz=0.0,
                  temperature=0.0, integrator=None, runsteps=220000,
                  thermosteps=100, dumpsteps=None, equilsteps=20000,
                  randomseed=None):
    """
    try:
        # Get script's location if __file__ exists
        script_dir = Path(__file__).parent
    except:
        # Use cwd otherwise
        script_dir = Path.cwd()

    # Get lammps units
    lammps_units = lmp.style.unit(potential.units)

    #Get lammps version date
    lammps_date = lmp.checkversion(lammps_command)['date']

    # Handle default values
    if dumpsteps is None:
        dumpsteps = runsteps

    # Define lammps variables
    lammps_variables = {}
    system_info = system.dump('atom_data', f='init.dat',
                              units=potential.units,
                              atom_style=potential.atom_style)
    lammps_variables['atomman_system_info'] = system_info
    lammps_variables['atomman_pair_info'] = potential.pair_info(system.symbols)
    integ_info = integrator_info(integrator=integrator,
                                 p_xx=p_xx, p_yy=p_yy, p_zz=p_zz,
                                 p_xy=p_xy, p_xz=p_xz, p_yz=p_yz,
                                 temperature=temperature,
                                 randomseed=randomseed,
                                 units=potential.units)
```





[1] C.A. Becker, F. Tavazza, Z.T. Trautt, and R.A. Buarque de Macedoc (2013) *Curr Opin Solid State Mater Sci*, **17**, 277-283.
[2] L.M. Hale, Z.T. Trautt, and C.A. Becker (2018) *Model Simul Mat Sci Eng*, **26**, 055003.
[3] S. Plimpton (1995) *J Comp Phys*, **117**, 1-19

# WHY ARCHIVE INTERATOMIC POTENTIAL FILES?

Easier to discover existing models - developing/training is time consuming

Newest is not “best” - different potentials trained for different conditions

Publications alone are often not enough to reproduce models

- Typos, errors and missing parameters
- Parameter rounding, numerical tabulations

Hosted models and their publications gain more exposure
(Submit models by emailing potentials@nist.gov)

# INTERATOMIC POTENTIALS REPOSITORY

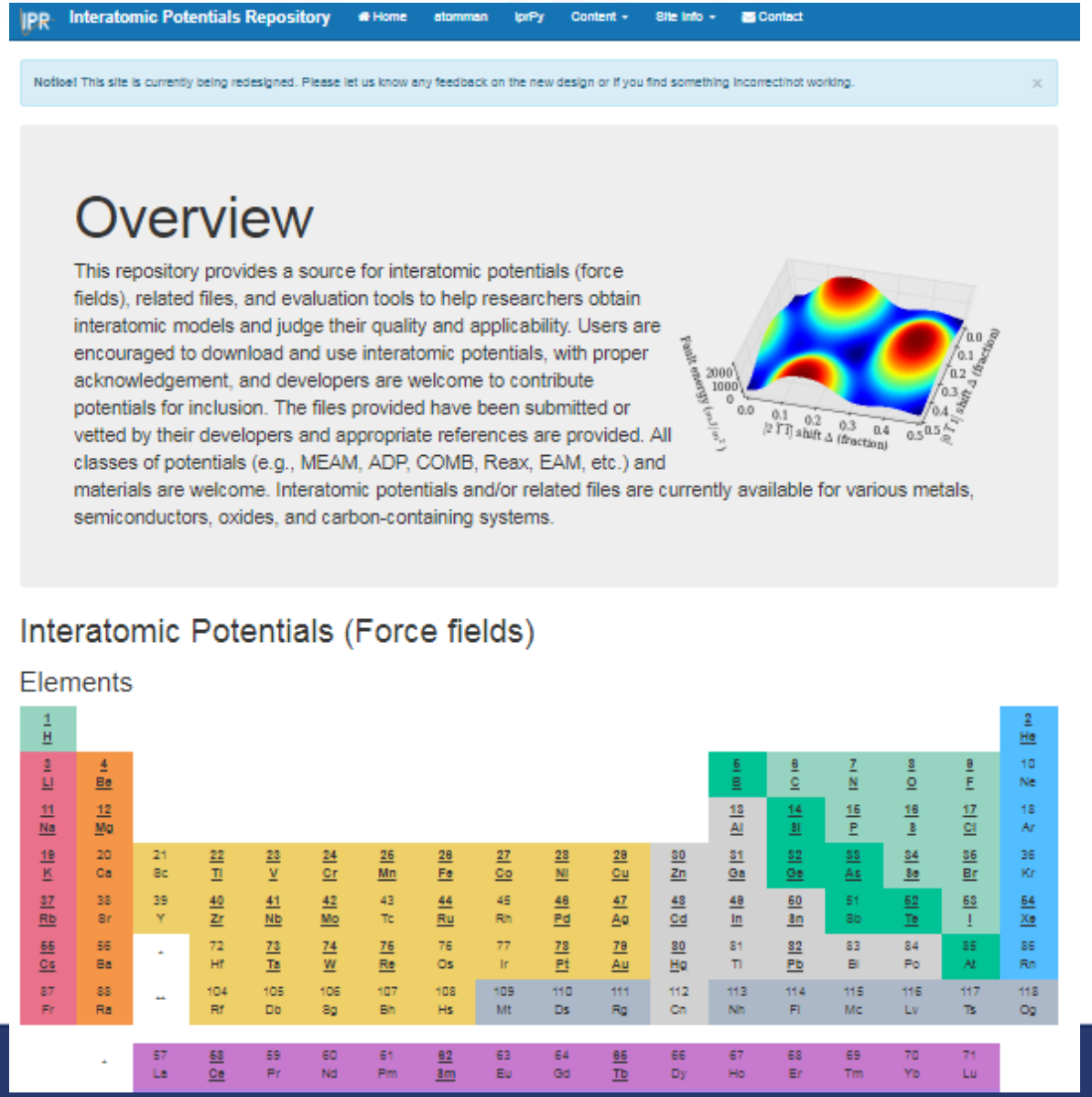
https://www.ctcms.nist.gov/potentials/

290+ potentials

- Known provenance
- Any format
  - EAM, MEAM, 3-Body, ML, reactive
  - FORTRAN, pdfs, LAMMPS mods
- Full citation and abstracts
- Can list potentials hosted elsewhere
- Property calculations

Incorporated into many projects

- OpenKIM
- JARVIS-FF
- Pyiron
- atomistictools.org
- MedeA



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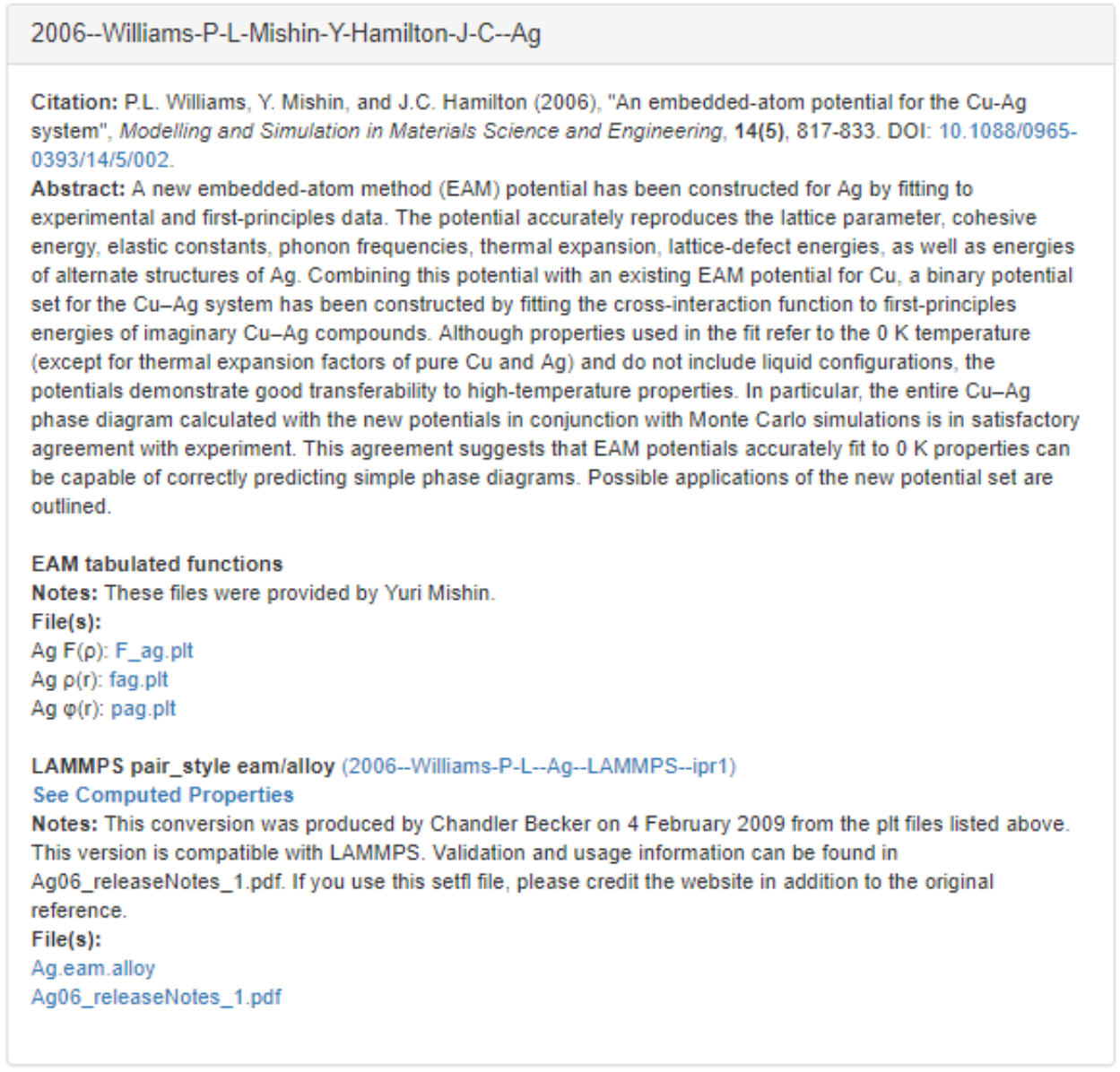


2006--Williams-P-L-Mishin-Y-Hamilton-J-C--Ag

**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(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

# PROPERTY CALCULATIONS

## 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. 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 whether the potential is suitable for radiation studies.

The calculation method used is available as the iprPy diatom_scan calculation method.

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**:

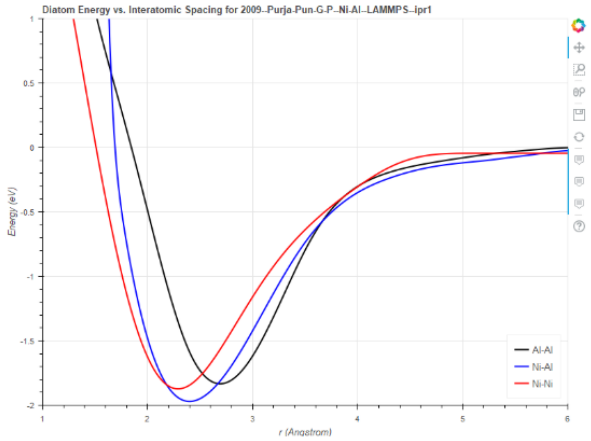
- These values are meant to be guidelines for comparing potentials, not the absolute values for any potential's properties. Values listed here may change if the calculation methods are updated due to improvements/corrections. Variations in the values may occur for variations in calculation methods, simulation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

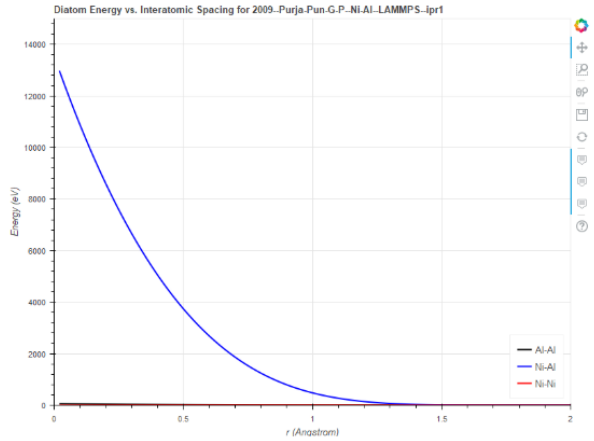
- 2019-11-14. Maximum value range on the shortrange plots are now limited to "expected" levels as details are otherwise lost.
- 2019-08-07. Plots added.

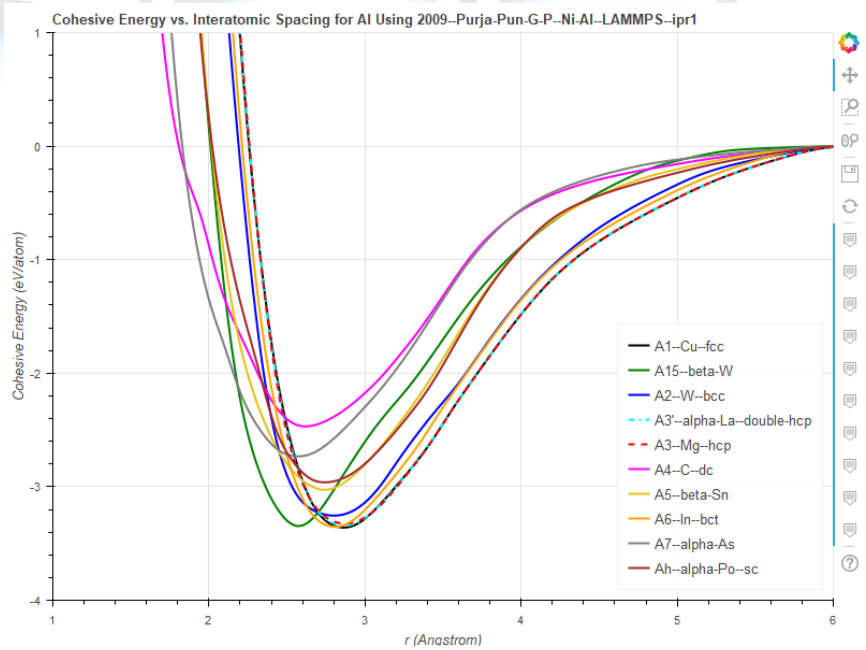
Download data

Click on plot to load interactive version




Click on plot to load interactive version

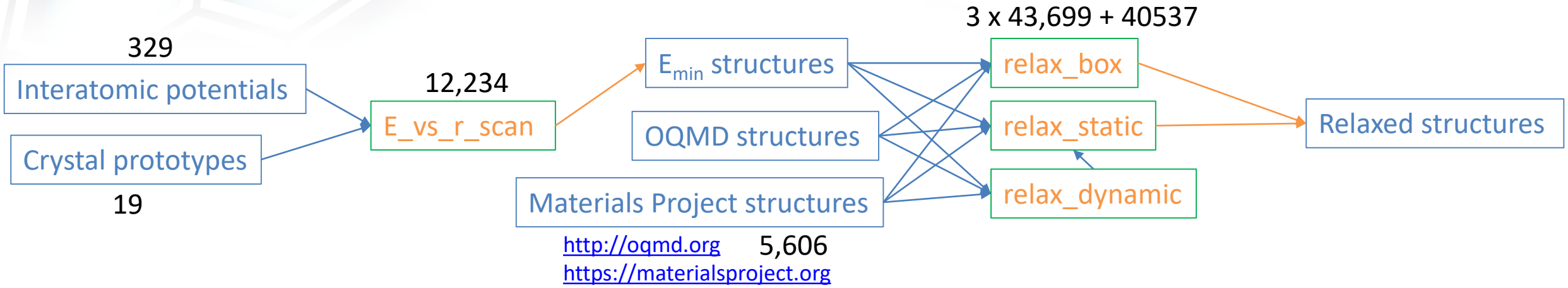


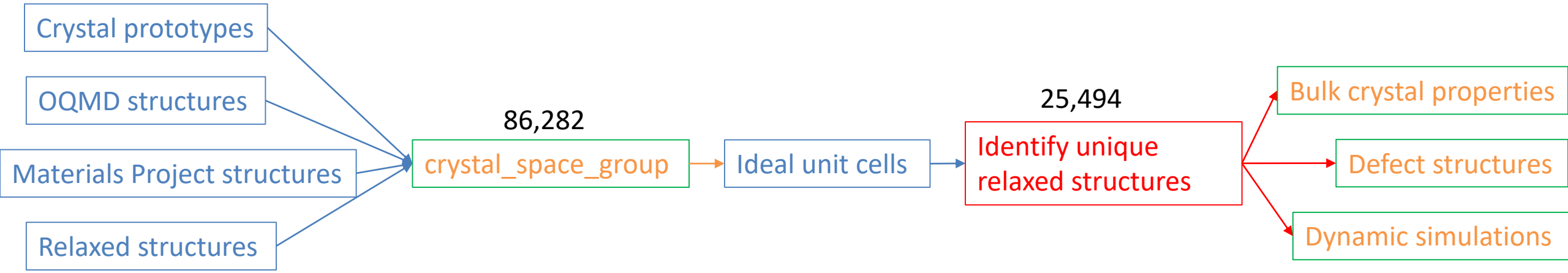




Reference structure matches:
A1--Cu--fcc = mp-23, oqmd-676148
A15--beta-W = oqmd-1214995
A2--W--bcc = mp-1008728, oqmd-22516
A3'--alpha-La--double-hcp = oqmd-1215441
A3--Mg--hcp = mp-10257, oqmd-677944
A5--beta-Sn = oqmd-1215619
A6--In--bct = oqmd-1215708

| prototype | method | $E_{coh}$ (eV) | $a_0$ (Å) | $b_0$ (Å) | $c_0$ (Å) | α (degrees) | β (degrees) | γ (degrees) |
|---|---|---|---|---|---|---|---|---|
| A1--Cu--fcc | dynamic | -4.45 | 3.52 | 3.52 | 3.52 | 90.0 | 90.0 | 90.0 |
| A3'--alpha-La--double-hcp | dynamic | -4.4387 | 2.4854 | 2.4854 | 8.1645 | 90.0 | 90.0 | 120.0 |
| oqmd-1216067 | static | -4.4351 | 2.4843 | 2.4843 | 18.4039 | 90.0 | 90.0 | 120.0 |
| A3--Mg--hcp | dynamic | -4.4279 | 2.4819 | 2.4819 | 4.1048 | 90.0 | 90.0 | 120.0 |
| A15--beta-W | dynamic | -4.4193 | 4.4342 | 4.4342 | 4.4342 | 90.0 | 90.0 | 90.0 |
| oqmd-1214906 | dynamic | -4.3975 | 6.0662 | 6.0662 | 6.0662 | 90.0 | 90.0 | 90.0 |
| oqmd-1214906 | box | -4.3971 | 6.0632 | 6.0632 | 6.0632 | 90.0 | 90.0 | 90.0 |
| oqmd-1214817 | dynamic | -4.3852 | 8.626 | 8.626 | 8.626 | 90.0 | 90.0 | 90.0 |
| oqmd-1214817 | box | -4.3835 | 8.6317 | 8.6317 | 8.6317 | 90.0 | 90.0 | 90.0 |
| A2--W--bcc | static | -4.3827 | 2.7687 | 2.7687 | 2.7687 | 90.0 | 90.0 | 90.0 |
| oqmd-1214728 | box | -4.0883 | 2.4659 | 2.4659 | 8.1654 | 90.0 | 90.0 | 90.0 |
| A5--beta-Sn | static | -3.8645 | 4.6612 | 4.6612 | 2.4242 | 90.0 | 90.0 | 90.0 |
| mp-1014111 | static | -3.8631 | 2.4596 | 2.4596 | 13.8025 | 89.1 | 88.9 | 60.0 |
| Ah--alpha-Po--sc | box | -3.7264 | 2.3965 | 2.3965 | 2.3965 | 90.0 | 90.0 | 90.0 |
| mp-1094136 | box | -3.5827 | 2.4434 | 4.2319 | 15.645 | 90.0 | 90.0 | 90.0 |
| oqmd-1215975 | box | -3.4255 | 3.8699 | 3.8699 | 3.9408 | 90.0 | 90.0 | 120.0 |
| A4--C--dc | static | -3.0336 | 5.2221 | 5.2221 | 5.2221 | 90.0 | 90.0 | 90.0 |

# RELAXED CRYSTALS WORKFLOW



# PROPERTY CALCULATIONS

Composition: Ni
Prototype: A5--beta-Sn
$a_0$: 4.661197976437832
strain: -1e-08
Download raw data

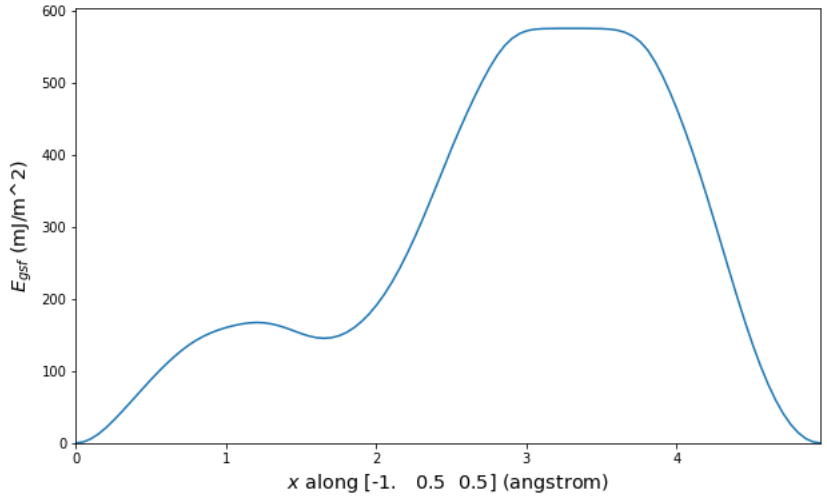
Cij in GPa:

| | | | | | |
|---|---|---|---|---|---|
| 196.217 | 10.274 | 28.433 | 0.0 | -0.0 | -0.0 |
| 10.274 | 196.217 | 28.433 | 0.0 | 0.0 | -0.0 |
| 28.433 | 28.433 | 208.03 | 0.0 | -0.0 | -0.0 |
| -0.0 | 0.0 | -0.0 | -47.194 | 0.0 | -0.0 |
| 0.0 | -0.0 | -0.0 | 0.0 | -47.194 | -0.0 |
| -0.0 | -0.0 | -0.0 | 0.0 | 0.0 | -36.496 |

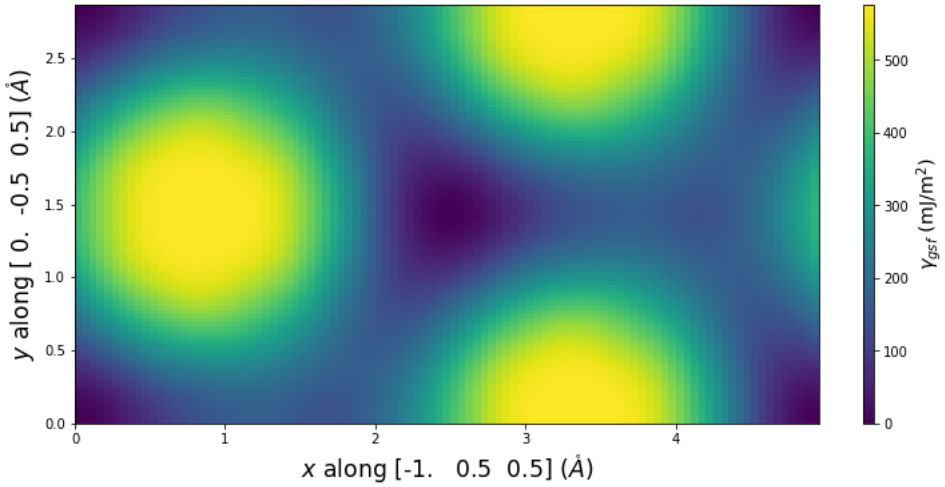
Composition: Al
Prototype: A1--Cu--fcc
$a_0$: 4.0499999995415665
Download raw data

| Surface | $\gamma_{fs}$ (mJ/m$^2$) |
|---|---|
| (331) | 1000.3 |
| (110) | 1006.03 |
| (311) | 1012.24 |
| (321) | 1026.58 |
| (310) | 1036.95 |
| (320) | 1043.01 |
| (210) | 1045.76 |
| (111) | 870.52 |
| (100) | 943.59 |
| (332) | 945.76 |
| (322) | 954.7 |
| (221) | 976.78 |
| (211) | 992.48 |

Composition: Al
Prototype: A1--Cu--fcc
$a_0$: 4.0499999995415665
plot: (111) [-1. 0.5 0.5]
Download raw data




Composition: Al
Prototype: A1--Cu--fcc
$a_0$: 4.0499999995415665
plot: (111)
Download raw data



# NEW! RELATED MODELS

Alloy potentials often use previously developed elemental interactions

Identifying families links models and can facilitate further development

“Related models” reveals the potentials that share effectively identical interactions

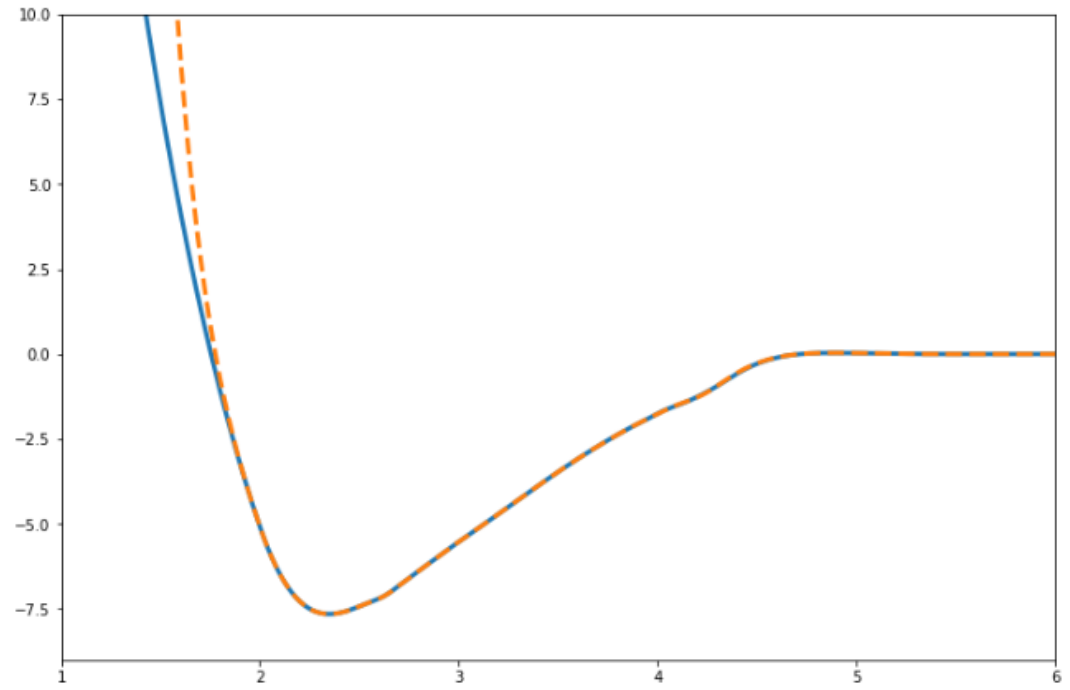
- Matches are identified by comparing diatom energy scans
- “Effective” ranges compared – small r repulsions and cutoffs may differ
- Automatic point-by-point comparisons cuts manual comparisons from 4500 to 50

**Related Models:**

- 2006--Williams-P-L-Mishin-Y-Hamilton-J-C--Cu-Ag (Ag)
- 2009--Wu-H-H-Trinkle-D-R--Cu-Ag (Ag)
- 2013--Hale-L-M-Wong-B-M-Zimmerman-J-A-Zhou-X-W--Pd-Ag-H-Hybrid (Ag)
- 2013--Hale-L-M-Wong-B-M-Zimmerman-J-A-Zhou-X-W--Pd-Ag-H-Morse (Ag)

```
73.80952380952381
2014--Bonny-G--W-H-He-2--LAMMPS--ipr1
2017--Bonny-G--W-Re--LAMMPS--ipr1

(-9.0, 10.0)
```



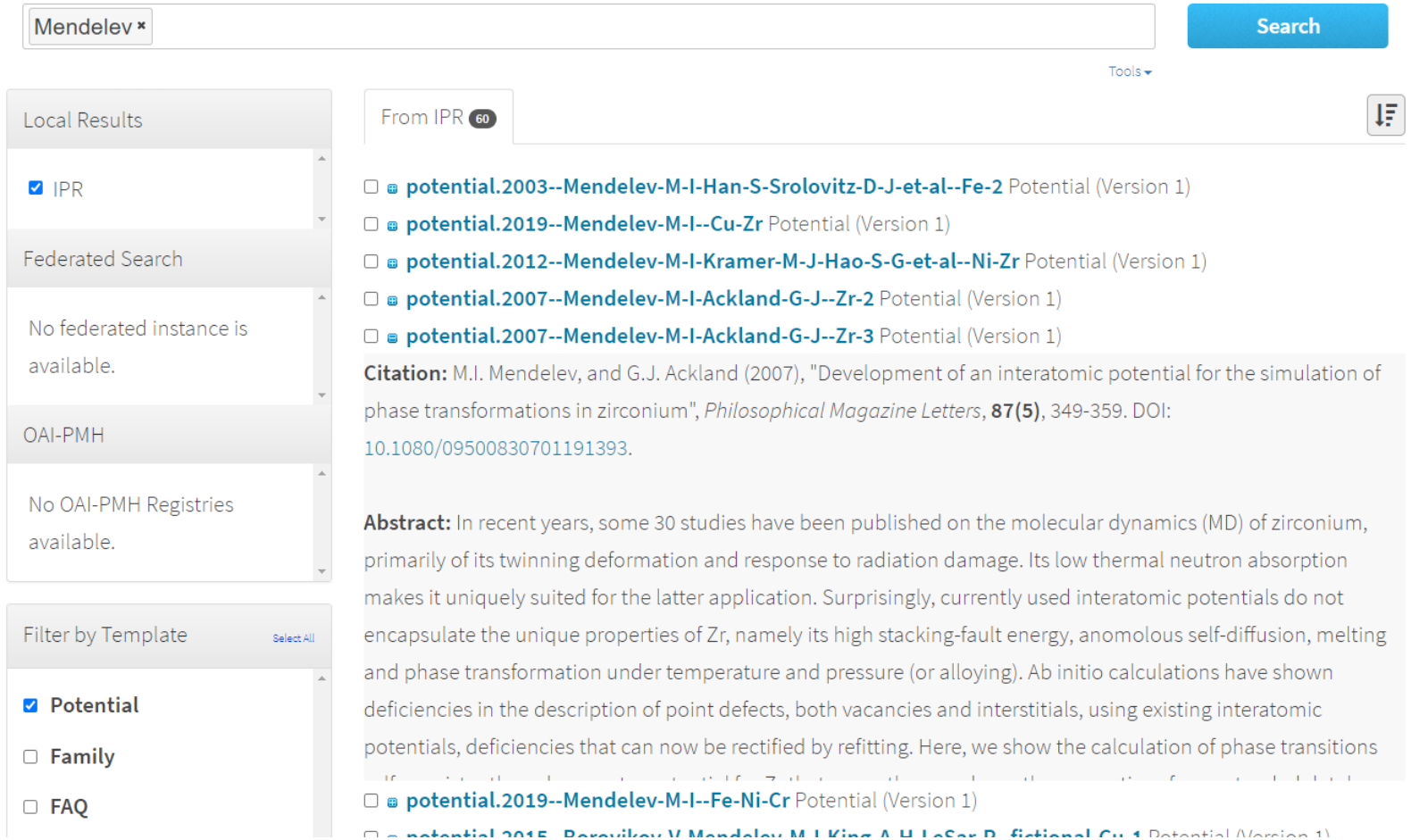
# HTTPS://POTENTIALS.NIST.GOV

Contains:

- Potentials listings
- Crystal prototypes
- Relaxed crystals
- Compiled properties
- Defect generation parameters
- Raw calc records (being added)

Explore using keywords or queries

Registered users can contribute



# POTENTIALS PYTHON PACKAGE

https://github.com/usnistgov/potentials

```
import potentials
```

```
potdb = potentials.Database(load='lammps_potentials', verbose=True)
```

```
Loaded 276 local LAMMPS potentials
Loaded 276 remote LAMMPS potentials
 - 0 new
```

```
potdb.lammps_potentials_df
```

| | id | key | potid | potkey | units | atom_style | allsymbols | pair_style | status | symbols | elements | masses | charges |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 1985--Foiles-S-M--Ni-Cu--LAMMPS--ipr1 | 062d2ba7-3903-40ae-a772-daa471d107c6 | 1985--Foiles-S-M--Ni-Cu | 301f04ce-9082-4542-8590-489300cd19e8 | metal | atomic | False | eam | active | [Cu, Ni] | [Cu, Ni] | [63.55, 58.71] | [0.0, 0.0] |
| 1 | 1985--Stillinger-F-H--Si--LAMMPS--ipr1 | d085648c-b3ef-4be8-824b-7093fd22770a | 1985--Stillinger-F-H-Weber-T-A--Si | edc31ad6-2b9a-455c-9b5f-e888a672ecbd | metal | atomic | False | sw | active | [Si] | [Si] | [28.085] | [0.0] |
| 2 | 1986--Foiles-S-M--Ag--LAMMPS--ipr1 | 76a265fc-45ff-49d7-8c64-2044f12402f2 | 1986--Foiles-S-M-Baskes-M-I-Daw-M-S--Ag | 672d54f8-9f48-4200-af56-8a7378ebbc4a | metal | atomic | False | eam | active | [Ag] | [Ag] | [107.87] | [0.0] |
| 3 | 1986--Foiles-S-M--Ag-Au-Cu-Ni-Pd-Pt--LAMMPS--ipr1 | c5afa7e8-6b3b-49cd-ad1c-ae3e4329363a | 1986--Foiles-S-M-Baskes-M-I-Daw-M-S--Ag-Au-Cu-... | 7a1302de-59cf-4efb-900e-cad845b68ee5 | metal | atomic | False | eam | active | [Ag, Au, Cu, Ni, Pd, Pt] | [Ag, Au, Cu, Ni, Pd, Pt] | [107.87, 196.97, 63.55, 58.71, 106.4, 195.09] | [0.0, 0.0, 0.0, 0.0, 0.0, 0.0] |
| 4 | 1986--Foiles-S-M--Au--LAMMPS--ipr1 | c588810a-b96d-4871-bfe2-cff8a5a7c709 | 1986--Foiles-S-M-Baskes-M-I-Daw-M-S--Au | ffb66faa-319d-4556-8363-dad3959cd553 | metal | atomic | False | eam | active | [Au] | [Au] | [196.97] | [0.0] |

Local directory

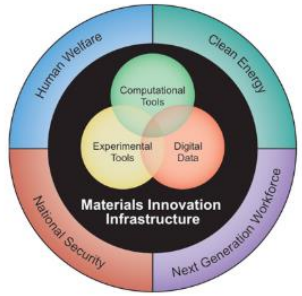
| Name | Date modified | Type |
|---|---|---|
| crystal_prototype | 3/25/2020 3:08 PM | File folder |
| dislocation | 3/25/2020 3:09 PM | File folder |
| free_surface | 3/31/2020 3:03 PM | File folder |
| point_defect | 3/25/2020 3:09 PM | File folder |
| potential_LAMMPS | 7/29/2020 2:45 PM | File folder |
| reference_crystal | 3/25/2020 3:40 PM | File folder |
| stacking_fault | 3/25/2020 3:09 PM | File folder |

https://potentials.nist.gov

## IPR Repository

This system allows for the curation of Material Data in a repository using predefined templates.

This is being developed at the National Institute of Standards and Technology and is made available to solicit comments from the Material Science community. Please do not enter any proprietary data into this system.



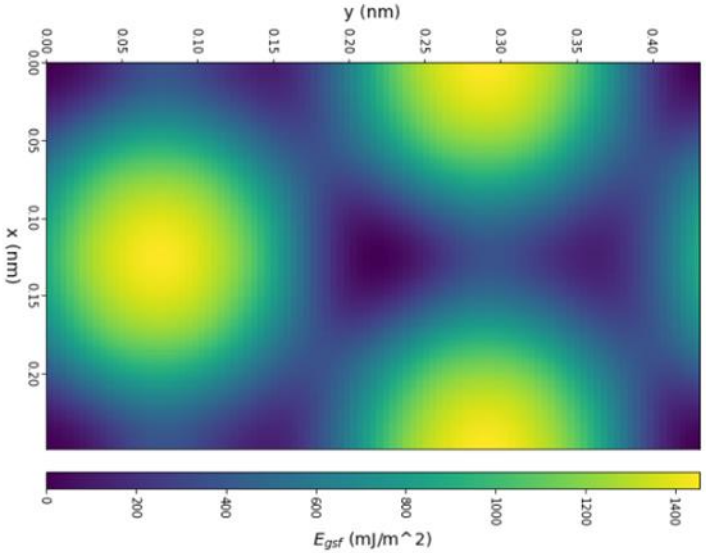
# ATOMMAN : ATOMISTIC MANIPULATION TOOLKIT

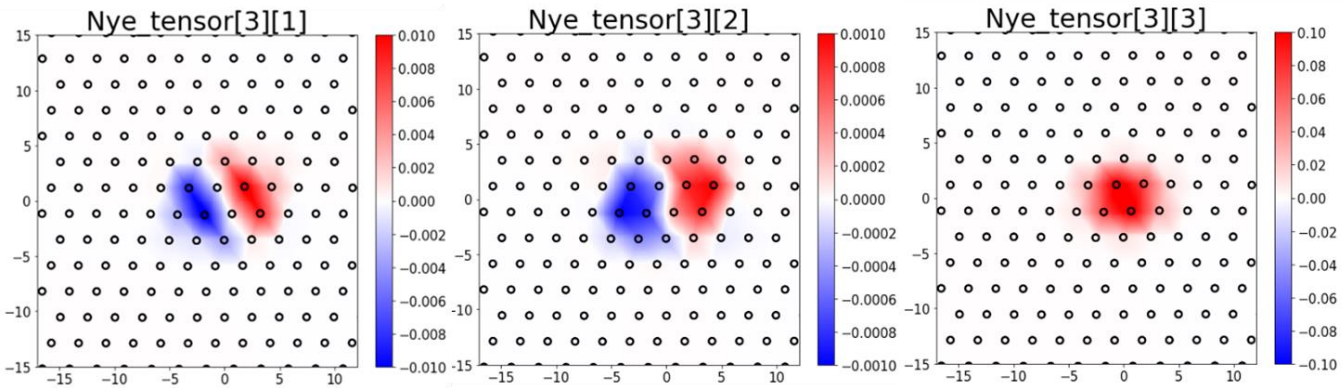
https://github.com/usnistgov/atomman

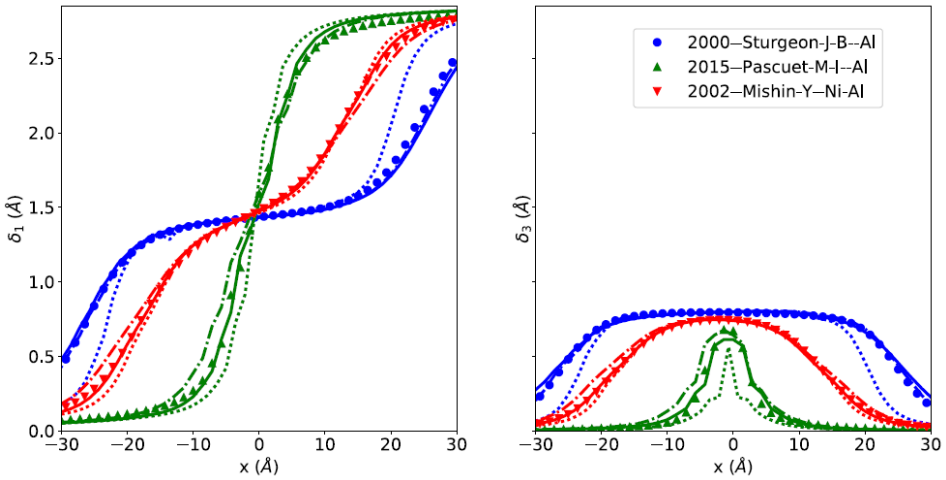
https://www.ctcms.nist.gov/potentials/atomman

Generic atomic representation designed to support large-scale classical atomistics

- Focus on defect generation + analysis
- Potential/simulator agnostic
- Built-in tools for interacting with LAMMPS



# ATOMMAN VS ASE AND PYMATGEN

Atomman was created for classical atomistic calculations rather than DFT

- Atom types, symbols and elements are not the same thing
    - Symbol indicates the interaction model
    - Some potentials have multiple symbols for the same element
    - Some symbols are not for explicit elements
    - Atom types can be assigned same or different symbols
- Atomic systems represent more than cells and molecules
    - Periodic boundary conditions can be changed
    - Cell box has origin position
- Per-atom properties can be freely assigned
    - Can be scalar, vector, or tensor values
    - Not built-in methods – can be calculated in any way
    - Atomic charges may be atom-specific or symbol-specific

But, atomman has built-in converters for atomman.System to/from ase.Atoms, pymatgen.Structure

# SOME BASIC ATOMMAN FEATURES

## Unit conversions

```
print('5.5 kg/(m*s^2) =')
pressure = uc.set_in_units(5.5, 'kg/(m*s^2)')

print(uc.get_in_units(pressure, 'Pa'), 'Pa')
```

```
5.5 kg/(m*s^2) =
5.5 Pa
```

## System rotations, multiplications

```
# Rotate system to crystal vectors [110], [-110], [001]
uvws = [[ 1, 1, 0],
        [-1, 1, 0],
        [ 0, 0, 1]]
system = system.rotate(uvws)

# Show system is transformed and expanded
print(system)
```

```
avect =  [ 5.728,  0.000,  0.000]
bvect =  [ 0.000,  5.728,  0.000]
cvect =  [ 0.000,  0.000,  4.050]
origin = [ 0.000,  0.000,  0.000]
natoms = 8
natypes = 1
symbols = ('Al',)
pbc = [ True  True  True]
per-atom properties = ['atype', 'pos']
     id   atype  pos[0]  pos[1]  pos[2]
      0       1   5.728   2.864   4.050
      1       1   0.000   0.000   4.050
      2       1   2.864   5.728   4.050
      3       1   1.432   1.432   2.025
      4       1   1.432   4.296   2.025
      5       1   2.864   2.864   4.050
      6       1   4.296   1.432   2.025
      7       1   4.296   4.296   2.025
```

## Neighbor lists

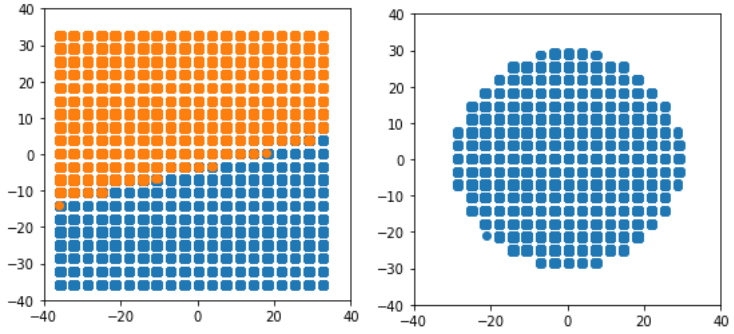
```
print('The neighbor atoms of atom 3 are', neighbors[3])
```

```
The neighbor atoms of atom 3 are [  2   4  22  24 202 204 222 224]
```

```
# The neighbor lists can also be iterated over for each atom
for nlist in neighbors:
    print(nlist)
    break
```

```
[   1   19  181  199 1801 1819 1981 1999]
```

## Geometric region selectors




## Miller-Cartesian conversions

```
indices = [[ 2/3,-1/3,-1/3, 0],
           [-1/3, 2/3,-1/3, 0],
           [   0,   0,   0, 1]]
print(am.tools.miller.vector_crystal_to_cartesian(indices, box))
```

```
[[ 2.51        0.          0.        ]
 [-1.255       2.17372376  0.        ]
 [ 0.          0.          4.07      ]]
```

## Elastic constants handling

**Cij** is the 6x6 Voigt representation.

[3]:
```
print('Cij (GPa) ->')
print(uc.get_in_units(C.Cij, 'GPa'))
```

```
Cij (GPa) ->
[[114.3  61.9  61.9   0.    0.    0. ]
 [ 61.9 114.3  61.9   0.    0.    0. ]
 [ 61.9  61.9 114.3   0.    0.    0. ]
 [  0.    0.    0.   31.6   0.    0. ]
 [  0.    0.    0.    0.   31.6   0. ]
 [  0.    0.    0.    0.    0.   31.6]]
```

**Cij9** is the full 9x9 representation.

[4]:
```
print('Cij9 (GPa) ->')
print(uc.get_in_units(C.Cij9, 'GPa'))
```

```
Cij9 (GPa) ->
[[114.3  61.9  61.9   0.    0.    0.    0.    0.    0. ]
 [ 61.9 114.3  61.9   0.    0.    0.    0.    0.    0. ]
 [ 61.9  61.9 114.3   0.    0.    0.    0.    0.    0. ]
 [  0.    0.    0.   31.6   0.    0.   31.6   0.    0. ]
 [  0.    0.    0.    0.   31.6   0.    0.   31.6   0. ]
 [  0.    0.    0.    0.    0.   31.6   0.    0.   31.6]
 [  0.    0.    0.   31.6   0.    0.   31.6   0.    0. ]
 [  0.    0.    0.    0.   31.6   0.    0.   31.6   0. ]
 [  0.    0.    0.    0.    0.   31.6   0.    0.   31.6]]
```

# DEFECT GENERATION AND ANALYSIS

Atomic configuration generators for

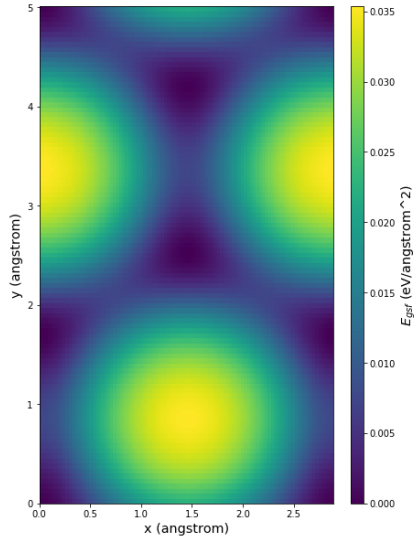
- Free surfaces
- Stacking faults
- Point defects
- Dislocations

Gamma surface class – point, 1D, 2D plots

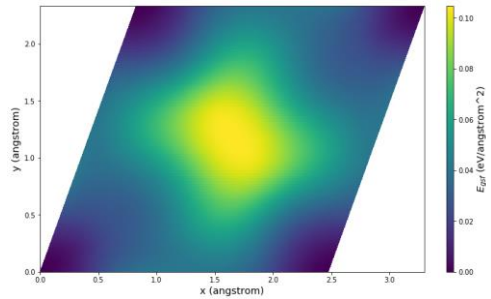
Dislocation structure analysis methods

- Disregistry
- Differential displacement
- Slip vector
- Nye tensor
- Semi-discrete Variational Peierls-Nabarro

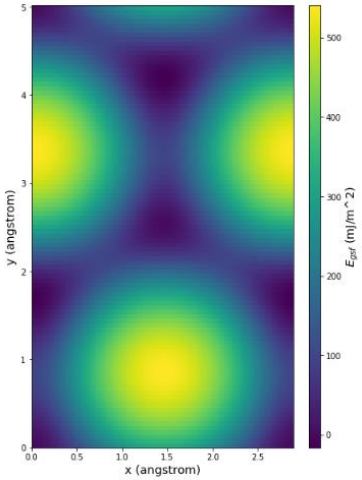
FCC (111)



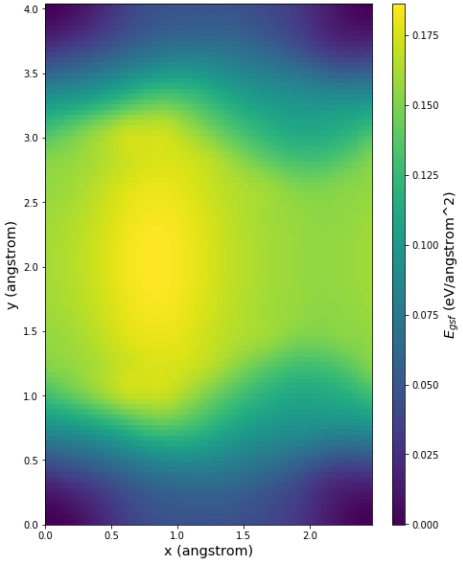

BCC (110)



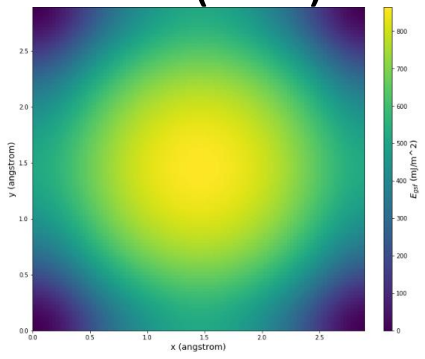

HCP (0001)



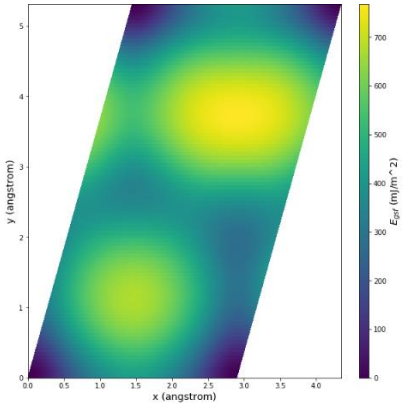

BCC (112)




FCC (100)




HCP (1011)



# POTENTIALS.NIST.GOV DATABASE ACCESSING

*NEW!* Atomman now uses potentials package – load potentials, prototypes and structures from database

## Load potential and relaxed crystal structure from database

```
potential = am.load_lammps_potential(id='2006--Williams-P-L--Ag--LAMMPS--ipr1')
print(potential)
```

```
2006--Williams-P-L--Ag--LAMMPS--ipr1
```

```
ucell = am.load('crystal', potential=potential, family='A1--Cu--fcc')
print(ucell)
```

```
avect =  [ 4.090,  0.000,  0.000]
bvect =  [ 0.000,  4.090,  0.000]
cvect =  [ 0.000,  0.000,  4.090]
origin = [ 0.000,  0.000,  0.000]
natoms = 4
natypes = 1
symbols = ('Ag',)
pbc = [ True  True  True]
per-atom properties = ['atype', 'pos']
     id |   atype |  pos[0] |  pos[1] |  pos[2]
      0 |       1 |   0.000 |   0.000 |   0.000
      1 |       1 |   0.000 |   2.045 |   2.045
      2 |       1 |   2.045 |   0.000 |   2.045
      3 |       1 |   2.045 |   2.045 |   0.000
```

# IPRPY CALCULATION FRAMEWORK

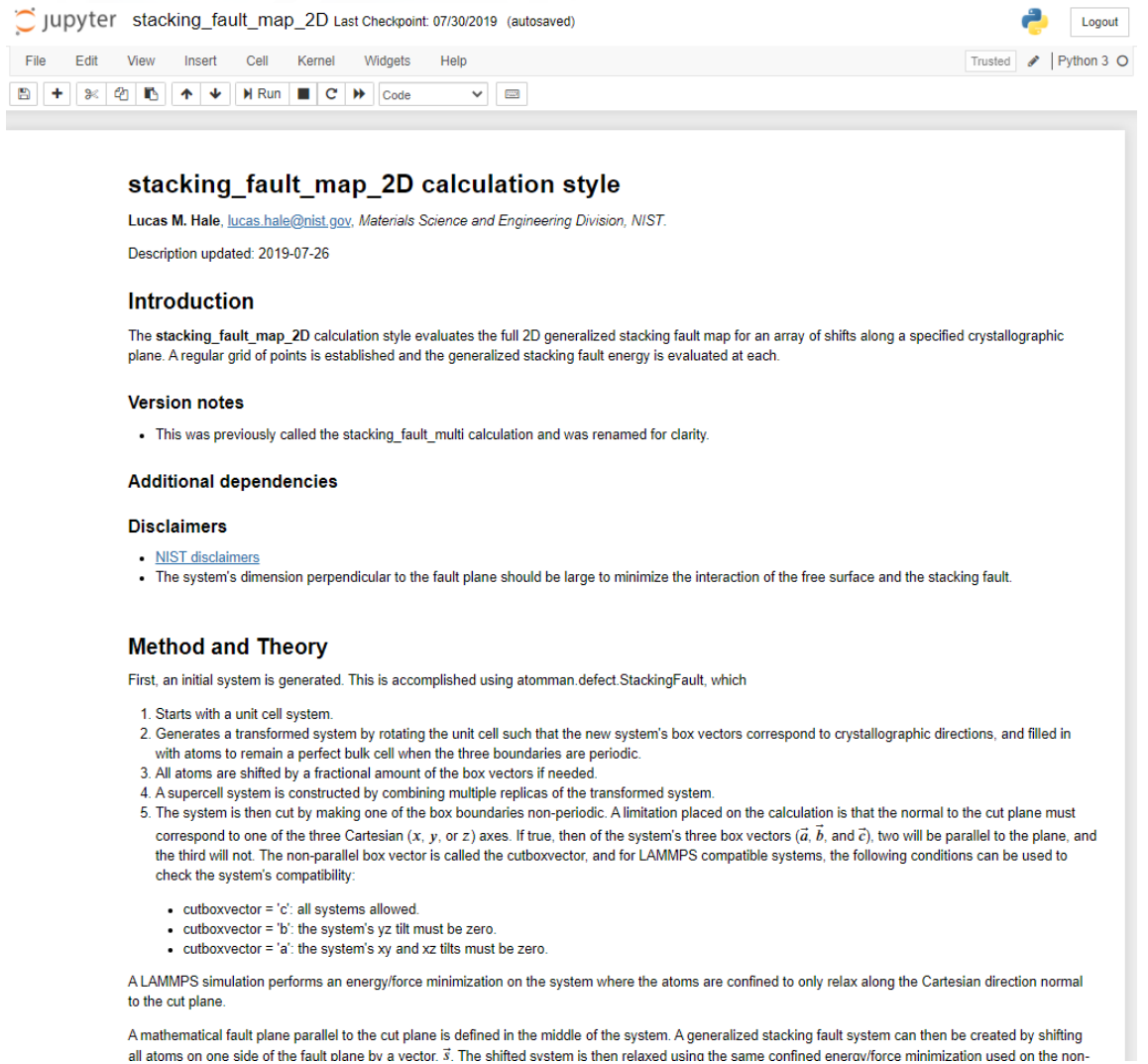
Property calculation methods with high-throughput tools

- 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 at all levels
- Transparent, documented methodologies
- Adaptable to new materials
- Transferable to other frameworks

Need data, but also need to *trust* the data!


jupyter stacking_fault_map_2D Last Checkpoint: 07/30/2019 (autosaved)

Logout

File Edit View Insert Cell Kernel Widgets Help

Trusted Python 3

Run Code

## stacking_fault_map_2D calculation style

**Lucas M. Hale**, lucas.hale@nist.gov, *Materials Science and Engineering Division, NIST.*

Description updated: 2019-07-26

### Introduction

The **stacking_fault_map_2D** calculation style evaluates the full 2D generalized stacking fault map for an array of shifts along a specified crystallographic plane. A regular grid of points is established and the generalized stacking fault energy is evaluated at each.

### Version notes

- This was previously called the stacking_fault_multi calculation and was renamed for clarity.

### Additional dependencies

### Disclaimers

- NIST disclaimers
- The system's dimension perpendicular to the fault plane should be large to minimize the interaction of the free surface and the stacking fault.

### Method and Theory

First, an initial system is generated. This is accomplished using atomman.defect.StackingFault, which

1. Starts with a unit cell system.
2. Generates a transformed system by rotating the unit cell such that the new system's box vectors correspond to crystallographic directions, and filled in with atoms to remain a perfect bulk cell when the three boundaries are periodic.
3. All atoms are shifted by a fractional amount of the box vectors if needed.
4. A supercell system is constructed by combining multiple replicas of the transformed system.
5. The system is then cut by making one of the box boundaries non-periodic. A limitation placed on the calculation is that the normal to the cut plane must correspond to one of the three Cartesian ($x$, $y$, or $z$) axes. If true, then of the system's three box vectors ($\vec{a}$, $\vec{b}$, and $\vec{c}$), two will be parallel to the plane, and the third will not. The non-parallel box vector is called the cutboxvector, and for LAMMPS compatible systems, the following conditions can be used to check the system's compatibility:

   - cutboxvector = 'c': all systems allowed.
   - cutboxvector = 'b': the system's yz tilt must be zero.
   - cutboxvector = 'a': the system's xy and xz tilts must be zero.

A LAMMPS simulation performs an energy/force minimization on the system where the atoms are confined to only relax along the Cartesian direction normal to the cut plane.

A mathematical fault plane parallel to the cut plane is defined in the middle of the system. A generalized stacking fault system can then be created by shifting all atoms on one side of the fault plane by a vector. $\vec{s}$. The shifted system is then relaxed using the same confined energy/force minimization used on the non-

# IMPLEMENTED CALCULATIONS

**Python script**: “black box” run from simple text input script

**Python class**: directly call underlying calculation methods

**Jupyter Notebook**: instructional “clear box” guide with description, code and example

**Workflows**: each is an independent unit of work

```
# 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
```

# IMPLEMENTED CALCULATIONS

**Python script**: “black box” run from simple text input script

**Python class**: directly call underlying calculation methods

**Jupyter Notebook**: instructional “clear box” guide with description, code and example

**Workflows**: each is an independent unit of work

```
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)
```

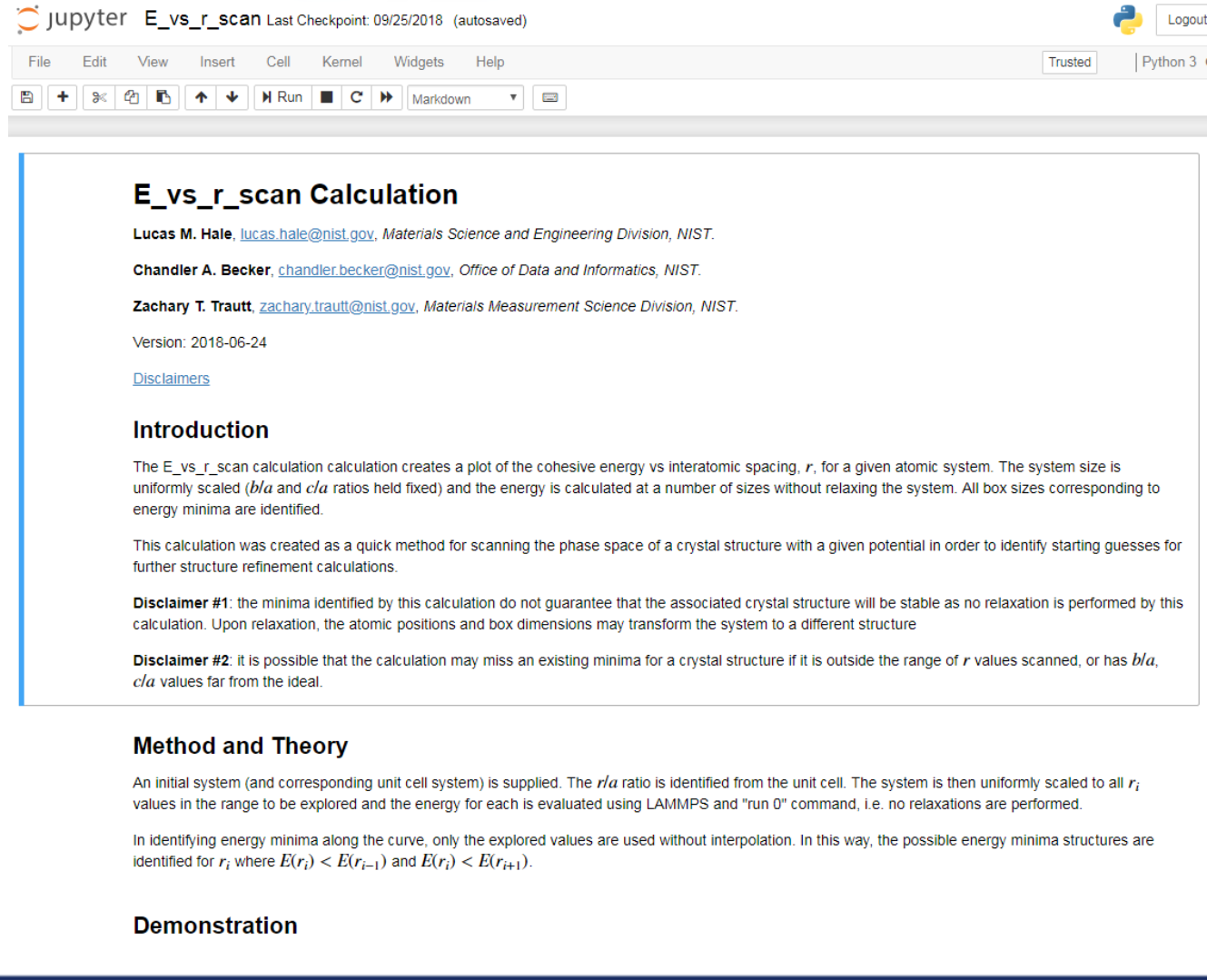
# IMPLEMENTED CALCULATIONS

**Python script**: “black box” run from simple text input script

**Python class**: directly call underlying calculation methods

**Jupyter Notebook**: instructional “clear box” guide with description, code and example

**Workflows**: each is an independent unit of work



# MODULAR METHOD DEVELOPMENT

Calculations, Records, Databases all modular subclasses – independent requirements

Modules for common inputs – faster development

```
# Input script for calc_E_vs_r_scan.py

# Command lines for LAMMPS and MPI
lammps_command            lmp_mpi
mpi_command

# Potential definition and directory containing associated files
potential_file            2004--Zhou-X-W--Pt--LAMMPS--ipr2.json
potential_dir             2004--Zhou-X-W--Pt--LAMMPS--ipr2

# Initial system configuration to load
load_file                 Al--Cu--fcc.json
load_style                system_model
load_options
family                    Al--Cu--fcc
symbols                   Pt
box_parameters

# System manipulations
a_uvw
b_uvw
c_uvw
atomshift
sizemults                 10 10 10

# Units for input/output values
length_unit
pressure_unit
energy_unit
force_unit

# Run parameters
minimum_r                 0.5
maximum_r                 6.0
number_of_steps_r         276
```

```
# Check lammps_command and mpi_command
iprPy.input.interpret('lammps_commands', input_dict)

# Load potential
iprPy.input.interpret('lammps_potential', input_dict)

# Load ucell system
iprPy.input.interpret('atomman_systemload', input_dict, build=build)

# Add atomic charges
iprPy.input.interpret('lammps_atomcharges', input_dict, build=build)

# Construct initialsystem by manipulating ucell system
iprPy.input.interpret('atomman_systemmanipulate', input_dict, build=build)
```

```
# Run e_vs_r
results_dict = e_vs_r(input_dict['lammps_command'],
                      input_dict['initialsystem'],
                      input_dict['potential'],
                      mpi_command = input_dict['mpi_command'],
                      ucell = input_dict['ucell'],
                      rmin = input_dict['minimum_r'],
                      rmax = input_dict['maximum_r'],
                      rsteps = input_dict['number_of_steps_r'])
```

```
"calculation-E-vs-r-scan": {
    "key": "036f4150-3936-48c6-8b8d-f0cce6e2dc47",
    "calculation": {
        "iprPy-version": "0.8.3",
        "atomman-version": "1.2.3",
        "LAMMPS-version": "5 Sep 2018",
        "script": "calc_E_vs_r_scan",
        "run-parameter": {
            "size-multipliers": {
                "a": [0, 10],
                "b": [0, 10],
                "c": [0, 10]},
            "minimum_r": {
                "value": 0.5,
                "unit": "angstrom"},
            "maximum_r": {
                "value": 6.0,
                "unit": "angstrom"},
            "number_of_steps_r": 276}},
    "potential-LAMMPS": {
        "key": "94afffa5-6a8d-4a97-a178-1412e65a2ffc",
        "id": "2004--Zhou-X-W--Pt--LAMMPS--ipr2",
        "potential": {
            "key": "b236a7be-023c-4df7-8146-da4fbdfcf900",
            "id": "2004--Zhou-X-W-Johnson-R-A-Wadley-H-N-G--Pt"}},
    "system-info": {
        "family": "Al--Cu--fcc",
        "artifact": {
            "file": "Al--Cu--fcc.json",
            "format": "system_model",
            "load_options": null},
        "symbol": "Pt"},
```

# PACKAGED CALCULATIONS (IN PROGRESS)

Pip install iprPy (conda coming soon)
GUI inputs (ipywidgets, nanoHUB, more?)
“Black box” and “clear box” versions

### 3. Calculation Input Parameters

- **LAMMPS**: LAMMPS executable to use
- **Potential**: Name of the interatomic potential to use
- **Symbol 1 and 2**: The elemental models from the potential to use for the two atoms
- **Min and Max r**: The range of interatomic distances to explore
- **Num r steps**: The number of measurements to make

```
input_dict = {}
widget_diatom_scan(input_dict)
```

LAMMPS: lmp_serial

Potential: 1998--Devanathan-R--Si-C--LAI

Symbol 1: Si

Symbol 2: C

Min r: 0.02

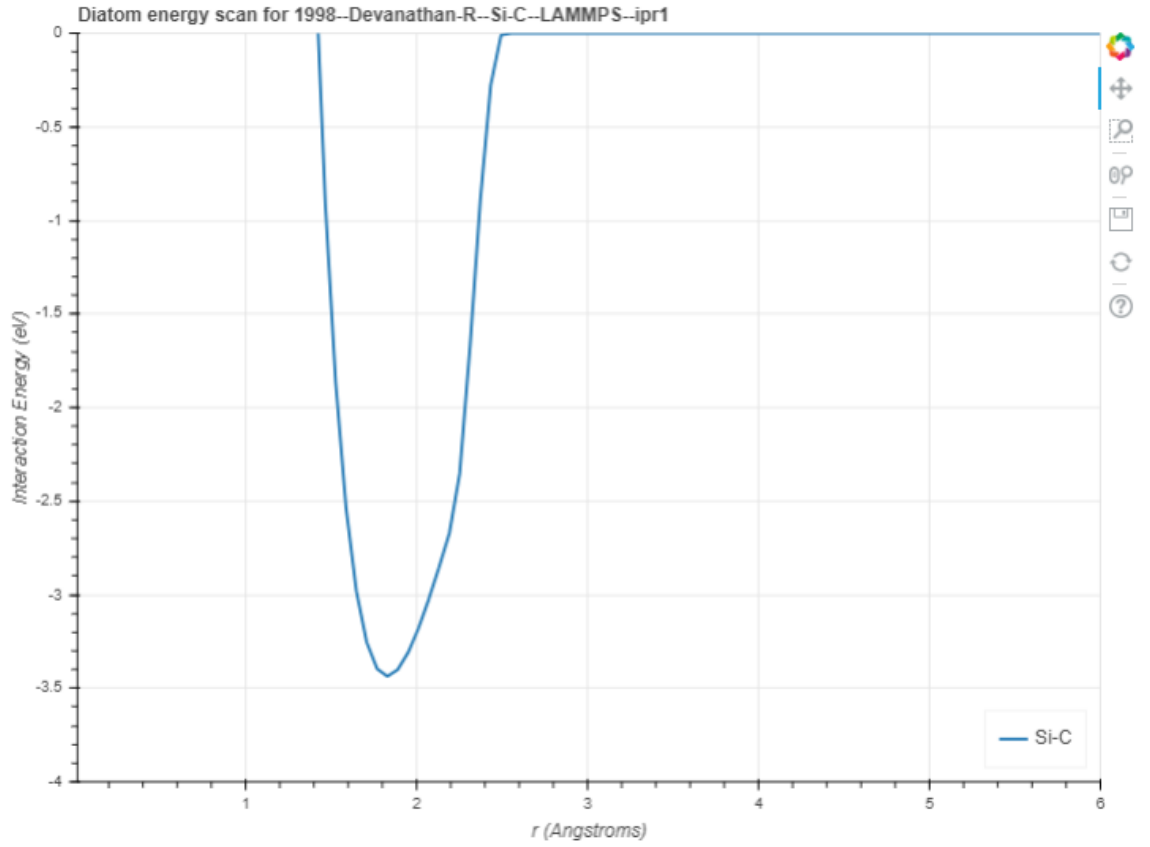
Max r: 6

Num r steps: 300

### 4. Run calculation function(s) and display results

```
results_dict = diatom(input_dict['lammps_command'],
                      input_dict['potential'],
                      input_dict['symbols'],
                      rmin = input_dict['rmin'],
                      rmax = input_dict['rmax'],
                      rsteps = input_dict['rsteps'])

show_E_vs_r_plot(input_dict, results_dict)
```



# JARVIS

https://www.ctcms.nist.gov/~knc6/JARVIS.html

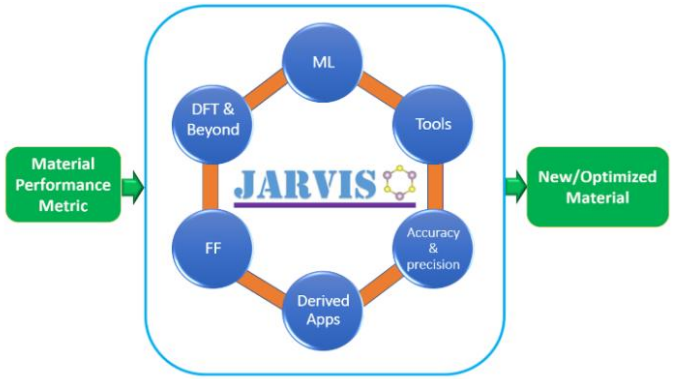
## JARVIS DFT

DFT database with
~40,000 3D materials
~1,000 2D materials

Primarily uses vdW-DF-OptB88 functional, and uses other beyond-GGA methods when needed

Conventional and unique datasets of property measurements

automatic k-point convergence protocol




## JARVIS FF

Database and framework for direct comparisons of classical potential properties to corresponding DFT results

## JARVIS ML

ML models based on DFT results to predict properties for “new” structures

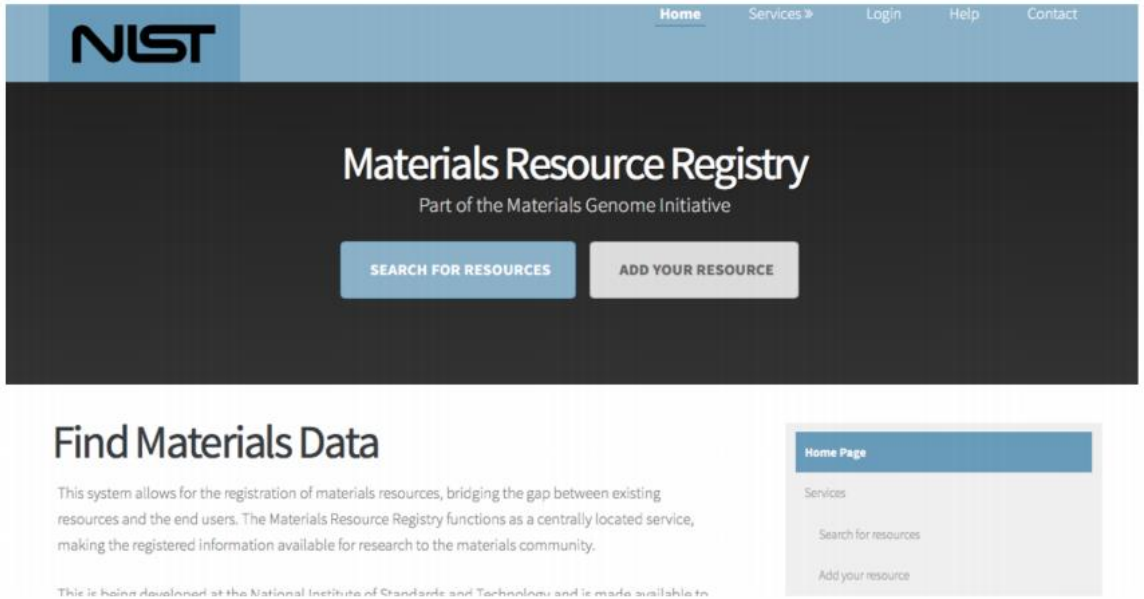
Used for fast materials-screening and energy-landscape mapping

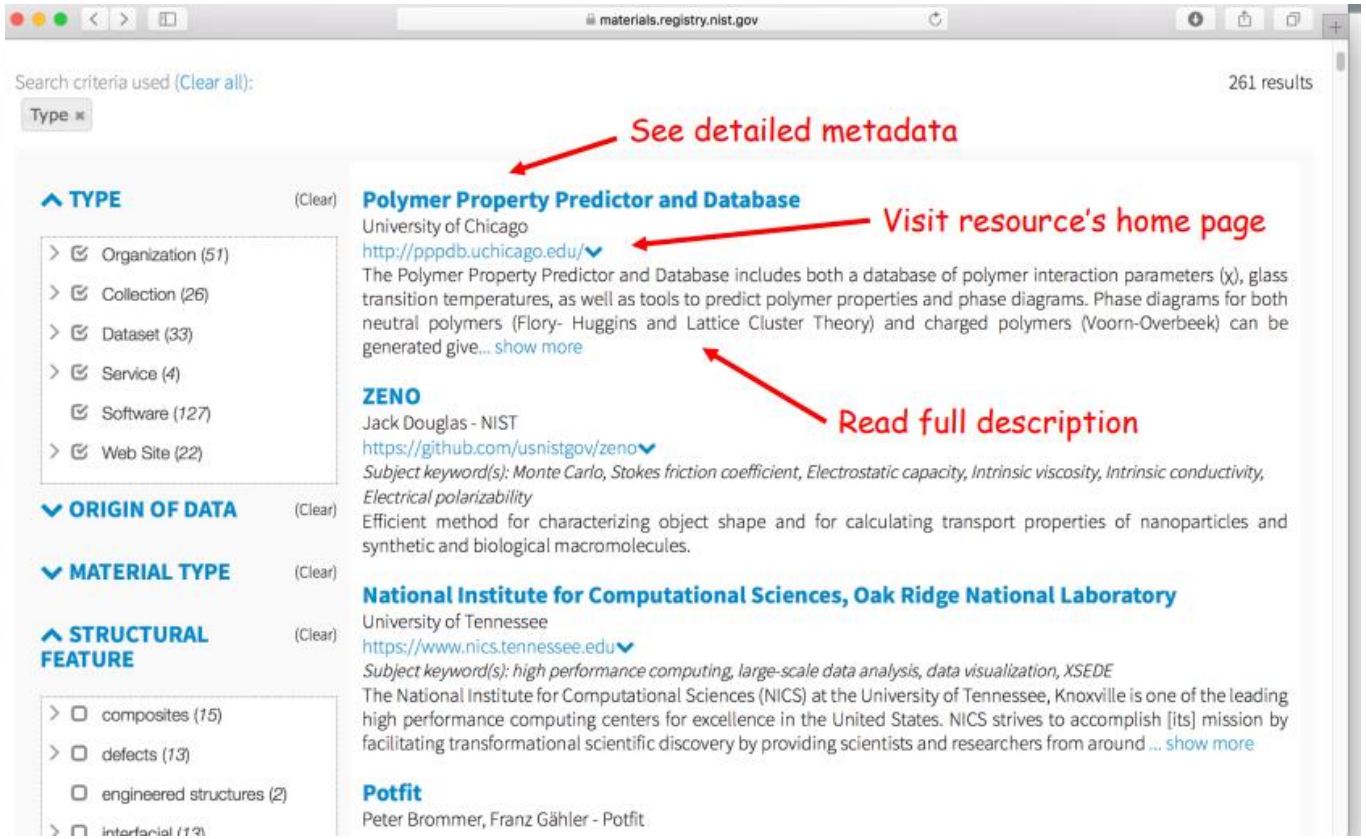
These models, the workflow, dataset etc. are disseminated to enhance the transparency of the work

JARVIS: An Integrated Infrastructure for Data-driven Materials Design, arXiv:2007.01831 (2020).

# MATERIALS RESOURCE REGISTRY

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



# LINKS

Interatomic Potentials Repository
https://www.ctcms.nist.gov/potentials/

Potentials database
https://potentials.nist.gov

Python potentials
https://github.com/usnistgov/potentials (stable)
https://github.com/lmhale99/potentials (development)

Python atomman
https://www.ctcms.nist.gov/potentials/atomman (documentation)
https://github.com/usnistgov/atomman (stable)
https://github.com/usnistgov/atomman (development)

Python iprPy
https://www.ctcms.nist.gov/potentials/iprPy (documentation)
https://github.com/usnistgov/iprPy (stable)
https://github.com/usnistgov/iprPy (development)

potentials, atomman and iprPy can be installed from code, pip, or conda-forge

Demonstrations of atomman and iprPy tomorrow at 10 AM