JARVIS: High Throughput Classical and Quantum Calculation Database for Materials

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

JARVIS-FF: Classical

$$F = ma = -\nabla V(r)$$

➢ **Approximations for V (force-fields)**:
EAM, EIM, MEAM, AIREBO, REAXFF, COMB, COMB3, TERSOFF, SW etc.

➢ **Goal of JARVIS-FF:**
- Evaluation of classical force-fields and provide easy user-interface,
- Comparison with DFT and experimental data
- Providing all the input files

➢ **Link**: http://www.ctcms.nist.gov/~knc6/periodic.html

➢ **Current status**:
- ***3583 calculations (>19000 sub-calculations) with LAMMPS***
- Version 1: Energetics, convex hull, elastic constants calculation
- Version 2: Addition of visualization of structure, vacancy formation energies, surface energies, phonon density of states and phonon band structure, visualization of phonons (under development phase)
- Now integrated in LAMMPS official website

NIST Disclaimer

Structural formula: Al

Force-field: Mishin-Ni-Al-2009.eam.alloy

Space group : Fm-3m

JARVIS ID: JLMP-1

Download input files

Elastic tensor (GPa)

Elastic tensor for the conventional cell of the system were calculated with LAMMPS in elastic script at 0 K. Similar script can be used for temperature dependent elastic constants and will be available here soon. WARNING! Please note that the starting lattice parameters of crystal structures were taken from density functional theory (DFT) and not from experiments. Generic minimization parameters were chosen for LAMMPS run rather than testing them for each individual case such as energy convergence criterion and so on. Hence, there are chances that the calculation gets trapped in a local energy minima. Please read carefully the assumptions taken during calculations in the in elastic script and use the data at your own risk

113.8	61.5	61.5	0.0	0.0	-0.0
61.5	113.8	61.5	0.0	-0.0	-0.0
61.5	61.5	113.8	0.0	-0.0	-0.0
0.0	0.0	0.0	31.6	-0.0	-0.0
0.0	-0.0	-0.0	-0.0	31.6	-0.0
-0.0	-0.0	-0.0	-0.0	-0.0	31.6

Vacancy-formation energy (eV)

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

Element	Mult.	Value
Al	4	0.674

Surface energy (J/m2)

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

Surface	Value
(1 1 1)	0.875
(1 0 0)	0.949
(3 3 2)	0.952
(3 2 2)	0.977
(2 1 1)	0.999
(3 3 1)	1.006
(3 1 0)	1.013
(3 1 1)	1.019
(3 2 1)	1.033
(3 1 0)	1.042
(3 2 0)	1.05
(2 1 0)	1.053
(3 3 1)	1.058

Phonon

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

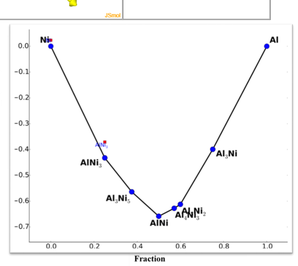
Visualize Phonons here

Phonon mode (cm^{-1}) Representation
-1.36864e-05 T1u I

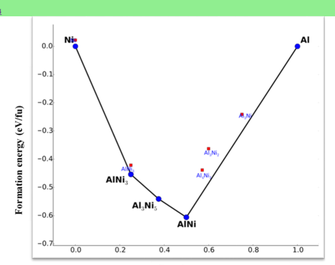
All phonon mode at Gamma point (cm^{-1})
-1.3874e-05
-1.2885e-05
-1.03024e-05
109.579415818
310.632537509

Reference

mp-134

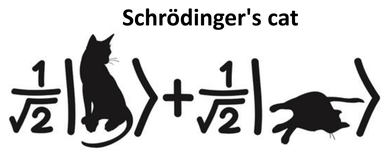


DFT (GGA-PBE)



FF (Mishin-NiAl-2009)

JARVIS-DFT : Quantum



$$H\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{Eff}(r)\right]\psi_i(r) = E_i(r)\psi_i(r)$$

$$V_{Eff} = T + V_{Ne} + V_{ee} + V_{XC}$$

➢ **Approximations for V_{XC} (Exchange-correlation):** LDA, PBE, vDW-DF, Hybrid etc.

➢ **Goal of JARVIS-DFT:**
- Identification of 2D bulk and multi-layer, Solar and Thermoelectric materials out of thousands of materials from databases
- Characterizing their properties
- Other DFT databases uses constant k-point, energy cut-off and PBE functionals, not suitable for 2D materials, we use vDW-DF
- Providing all the input files
- Effect of XC on properties

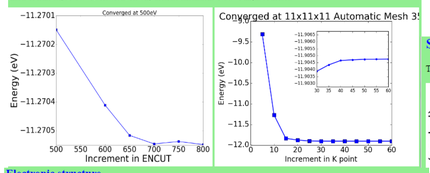
➢ **Link**: http://www.ctcms.nist.gov/~knc6/JVASP.html

➢ **Current status**: *(under development phase)*

873 calculations (>25000 sub-calculations) with VASP

Convergence

Calculations are done using VASP software. Convergence on KPOINTS and ENCUT is done with respect to total energy of the system within 0.001 eV tolerance. Please note convergence on KPOINTS and ENCUT is generally done for target properties, but here we assume energy-convergence with 0.001 eV should be sufficient for other properties also. The points on the curves are obtained with single-point calculation (number of ionic steps:NSW=1). However, for very accurate calculations, NSW=1 might be needed.



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Structural formula: Si2

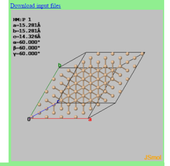
Functional: LDA

Space group : Fd-3m

Calculation type: Bulk

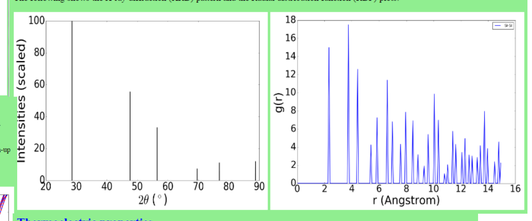
JARVIS ID: JVASP-94

Download input files



Structural analysis

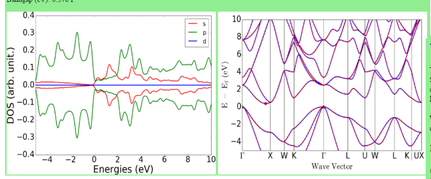
The following shows the X-ray diffraction (XRD) pattern and the Radial distribution function (RDF) plots.



Electronic structure

The following shows the electronic density of states and bandstructure. DFT is generally predicted to underestimate bandgap of materials. Accurate band-gaps are obtained with higher level methods (with high computational requirement) such as HSE, GW, which are under progress. Total DOS, Orbital DOS and Element dos buttons are provided for density of states options. Energy is rescaled to make Fermi-energy zero. In the bandstructure plot, spin up is is shown with blue lines while spin down are shown with red lines. Non-degenerate spin-up and spin-down states (if applicable) would imply a net orbital magnetic moment in the system.

Bandgap (eV): 0.376 I



Elastic tensor and derived phonon properties

Elastic tensor calculated for the conventional cell of the system with finite-difference method. For layered materials, the elastic constants are rescaled with respect to vacuum padding (see the input files) and the units for elastic coefficients are in N/m. Phonons obtained from this calculation are also shown.

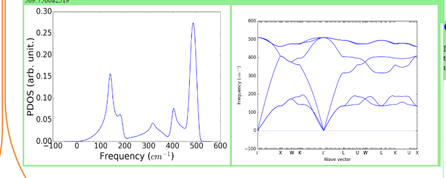
WARNING: Please note this may not be the exact phonon modes of the system as we did not test the cell-size dependence of phonons yet. At least 1.2 nm x1.2 nm x1.2 nm or more is needed for obtaining reliable phonon spectrum. For systems having primitive-cell phonon representation tables, I denotes infrared activity and R denotes Raman active modes (where applicable).

Elastic Tensor C_{ij} GPa

159.6	65.1	65.1	0.0	0.0	0.0
65.1	159.6	65.1	0.0	0.0	0.0
65.1	65.1	159.6	0.0	0.0	0.0
0.0	0.0	0.0	75.0	0.0	0.0
0.0	0.0	0.0	0.0	75.0	0.0
0.0	0.0	0.0	0.0	0.0	75.0

Phonon mode (cm^{-1}) Representation
3.8853e-06 T1u I
499.516824396 T2g R

Phonon mode (cm^{-1})
-0.0521466365
-0.0521466361
-0.0521466347
136.239760177
408.173817129
460.782147546
509.756683519



Thermoelectric properties

Thermoelectric properties are calculated using BoltzTrap code. Electron and hole mass tensors are given at 300 K. Following plots show the Seebeck coefficient and ZT factor (eigenvalues of the tensor shown) at 300 K along three different crystallographic directions. Seebeck coefficient and ZT plots can be compared for three different temperatures available through the buttons given below. Generally very high Kpoints are needed for obtaining thermoelectric properties. We assume the Kpoints obtained from above convergence were sufficient.

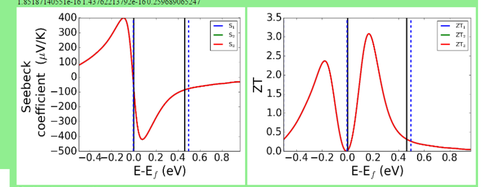
WARNING: Constant relaxation time approximation (10^{-14} s) and only electronic contribution to thermal conductivity were utilized for calculating ZT.

Electron mass tensor (m_e unit)

0.213343254384	7.30501044958e-17	1.8189090980	4e-16
7.30501044958e-17	0.213342672914	1.38823476056	e-16
1.8189090980	4e-16	1.38823476056e-16	0.213342995953

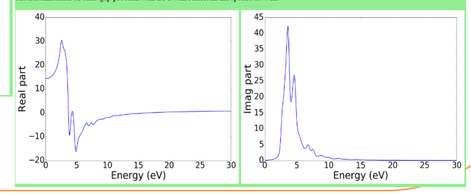
Hole mass tensor (m_e unit)

0.259689400293	6.595116759	92e-17	1.8518714055	1e-16
6.595116759	92e-17	0.259688682339	1.437622137	92e-16
1.8518714055	1e-16	1.437622137	92e-16	0.259689065247

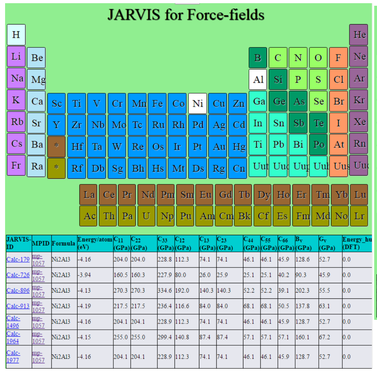


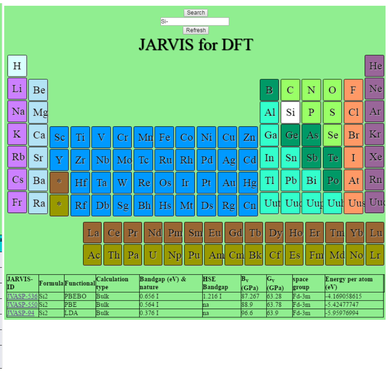
Optical properties

Incident photon energy dependence of real and imaginary part of dielectric function is shown below. Only interband optical transitions are taken into account. Absorption, reflectivc, transmittance spectra and Drude-Lorentz parameters will be available soon. Please note the underestimatation of band-gap problem with DFT will reflect in the spectra as well.

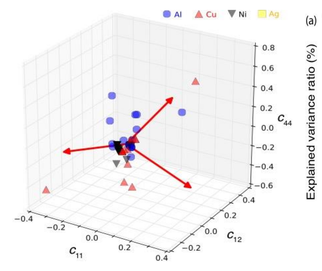


Easy Web-interface

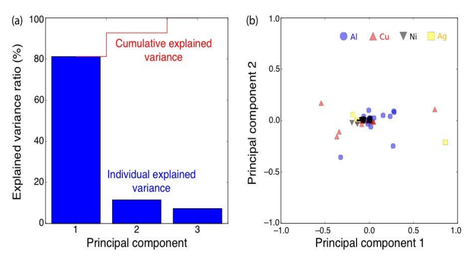




Implementation of Machine Learning Tools



Relative error in C_{ij}



PCA analysis

Ongoing work

- JARVIS-ONE: Tools to accumulate and compare various DFT, FF and experimental data in one web-interface
- JARVIS-FF: Thermal conductivity, genetic algorithm evaluation, stacking fault, grain-boundary energies calculations
- JARVIS-DFT: 2L, 3L, 4L structures for 2D materials, comparison of solar cell material and thermoelectric properties performance, HSE band-structures calculations
- Implementation of voice-recognition based query tools and better machine learning tools

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