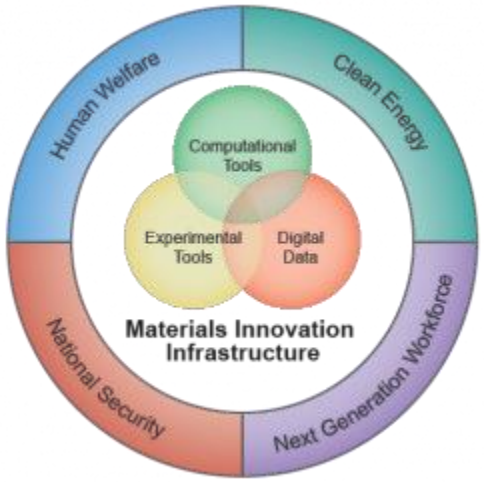


JARVIS-DFT

Quantum calculation database for 2D, Solar-cell and Thermoelectric materials

NIST Materials Genome Initiative
Gateway to Materials Genome Information

What is JARVIS-DFT?

JARVIS-DFT is a **density functional theory** (DFT) calculation database for **2D materials, solar cells and thermoelectric**.

At present, the database consists of **873 DFT calculations (>25000 sub-calculations)** for **energetics**, **structural properties** (computational X-ray diffraction, radial distribution function), **electronic properties** (density of states, band-structure), **elastic properties** (modulus of elasticity, associated phonon, its representation and visualization) , **optical properties** (dielectric function, absorption spectra, refractive index) and **thermoelectric properties** (Seebeck coefficient, ZT-factor, effective mass of charge-carriers).

All the calculations were done with VASP software. Some of the key-features for JARVIS-DFT are:

1) We used the **vDW-DF functional,** which works better for 2D materials than PBE or other commonly used functionals;
2) The database contains **both 2D-layered and 2D-bulk structure data** (for comparison) and we used a **tighter DFT convergence criteria** than other databases.
3) JARVIS-DFT was made with custom-modification of the publicly available Pymatgen, Phonopy and ASE tools. We greatly appreciate these tools.
4) To enhance **data-reproducibility, all data** in the database, as well as all the **metadata** (input files etc.) needed to reproduce the results are **available for download** from the website

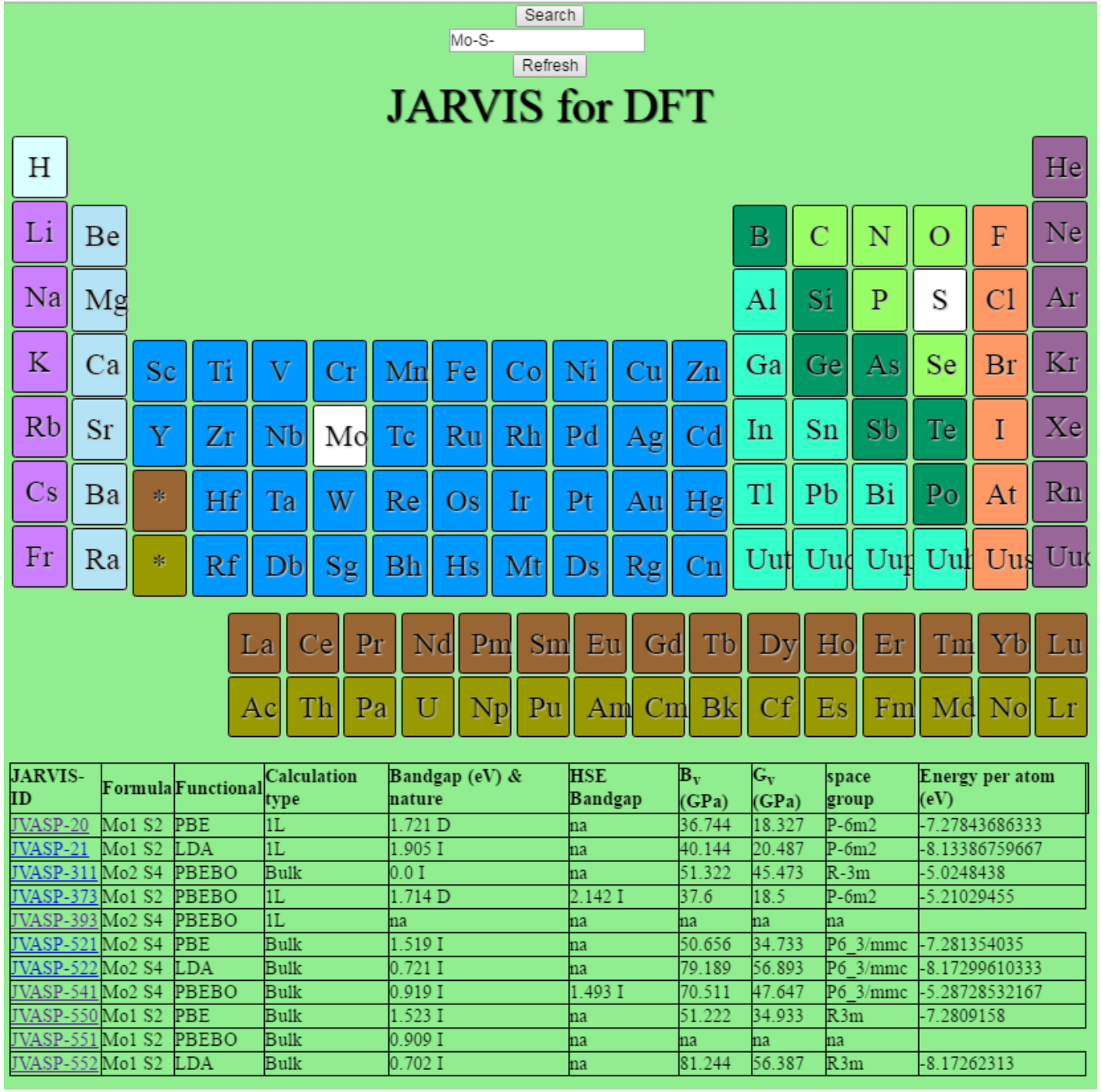
http://www.ctcms.nist.gov/~knc6/JVASP.html

Methodology

1. Crystal structure: Crystal structures were obtained from publicly available DFT-repositories such as **Materials project, AFLOW and OQMD** based on criteria for 2D materials. Single-layer counterparts were created manually from these structures.

2. High-throughput calculations: We compute optimized energy cut-off and K-point sampling within tolerance of 0.001 eV. After that full ionic and electronic relaxation were carried out. After relaxation properties such as elastic calculations, optical properties and band-structures were calculated in next set of calculations. Automatic error-checking and error-correction features were included in JARVIS-DFT.

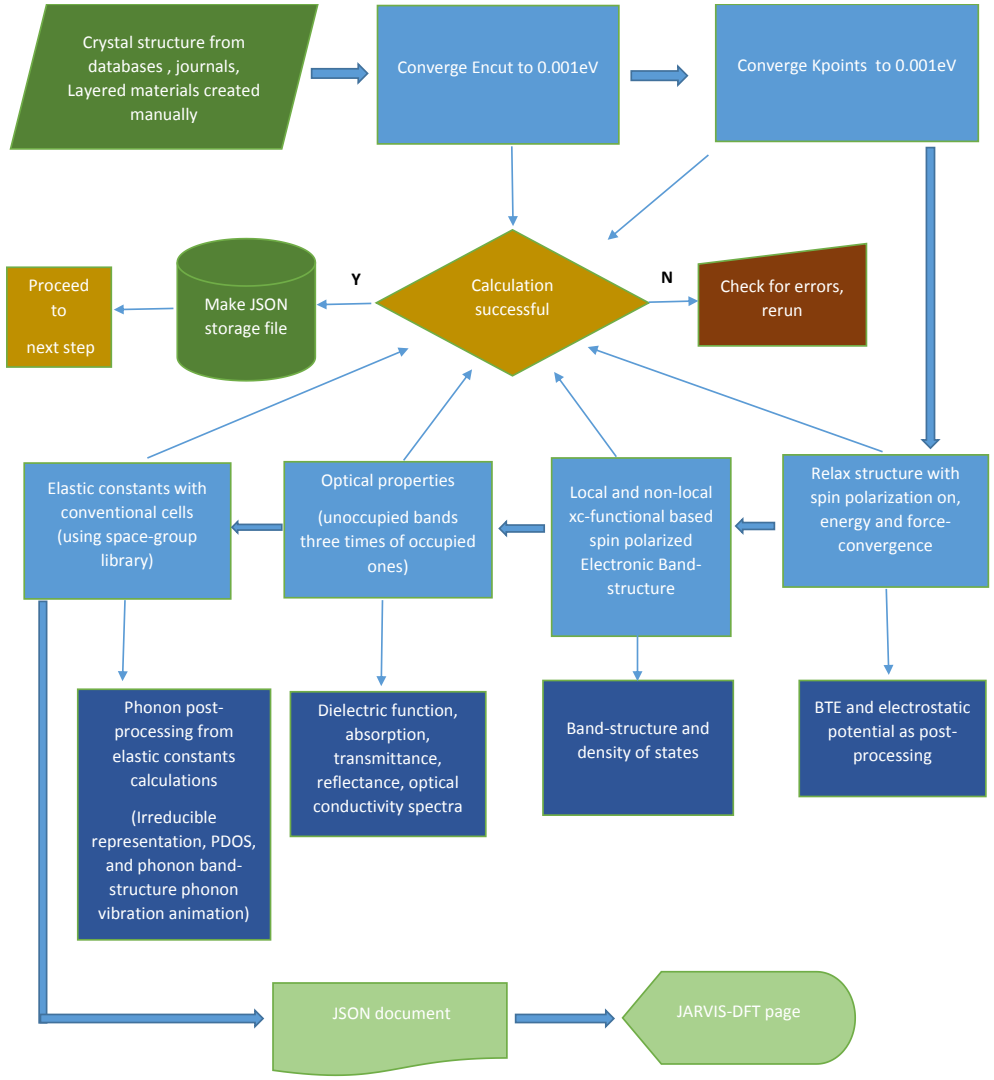
3. User-interface: MongoDB for all the calculation data were prepared and then an interactive periodic table was constructed for all the calculations. We also provide materials project, AFLOW and ICSD links wherever applicable.



JARVIS-ID	Formula	Functional	Calculation type	Bandgap (eV) & nature	HSE Bandgap	B_V (GPa)	G_V (GPa)	space group	Energy per atom (eV)
JVASP-20	Mo1 S2	PBE	1L	1.721 D	na	36.744	18.327	P-6m2	-7.27843686333
JVASP-21	Mo1 S2	LDA	1L	1.905 I	na	40.144	20.487	P-6m2	-8.13386759667
JVASP-311	Mo2 S4	PBEBO	Bulk	0.0 I	na	51.322	45.473	R-3m	-5.0248438
JVASP-373	Mo1 S2	PBEBO	1L	1.714 D	2.142 I	37.6	18.5	P-6m2	-5.21029455
JVASP-393	Mo2 S4	PBEBO	1L	na	na	na	na	na	
JVASP-521	Mo2 S4	PBE	Bulk	1.519 I	na	50.656	34.733	P6_3/mmc	-7.281354035
JVASP-522	Mo2 S4	LDA	Bulk	0.721 I	na	79.189	56.893	P6_3/mmc	-8.17299610333
JVASP-541	Mo2 S4	PBEBO	Bulk	0.919 I	1.493 I	70.511	47.647	P6_3/mmc	-5.28728532167
JVASP-550	Mo1 S2	PBE	Bulk	1.523 I	na	51.222	34.933	R3m	-7.2809158
JVASP-551	Mo1 S2	PBEBO	Bulk	0.909 I	na	na	na	na	
JVASP-552	Mo1 S2	LDA	Bulk	0.702 I	na	81.244	56.387	R3m	-8.17262313

Fig.1: Main components of the web user interface

Technical details



- First we extract crystal structures from **DFT databases** and **journals repository** for bulk-structures, then, for most of them, we manually created the layered structures;
- JARVIS-DFT obtains **optimized energy-cut-off and K-point** based on series of runs. We impose **force-convergence criteria** in addition to energy-convergence.
- After main-relaxation, **optical, elastic, phonon, thermoelectric, band-structure and magnetic property** calculations are performed. **Automatic error-check** and error-corrections are implemented. On the website we provide details on all the assumptions used in calculations.
- All the data is saved in **JSON** format making a main MongoDB for JARVIS-DFT.
- The interactive website is constructed with HTML5 and JavaScript.

NIST Disclaimer

Structural formula: Si2

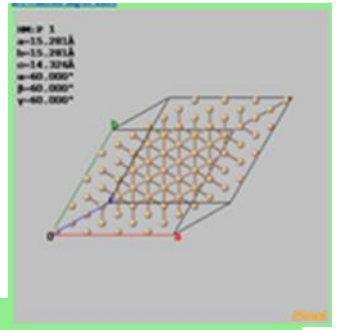
Functional: LDA

Space group : Fd-3m

Calculation type: Bulk

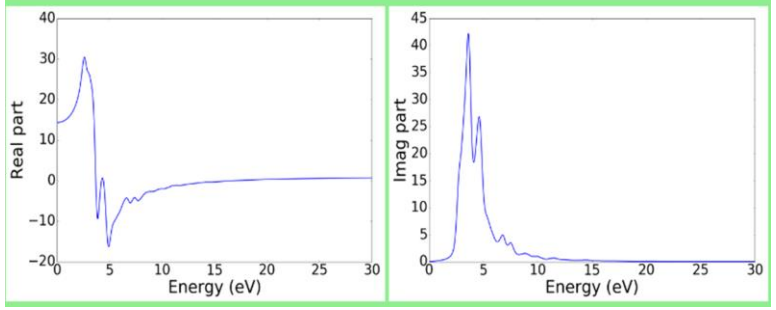
JARVIS ID: JVASP-94

Examples of computed quantities



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, reflectanc, 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.



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.

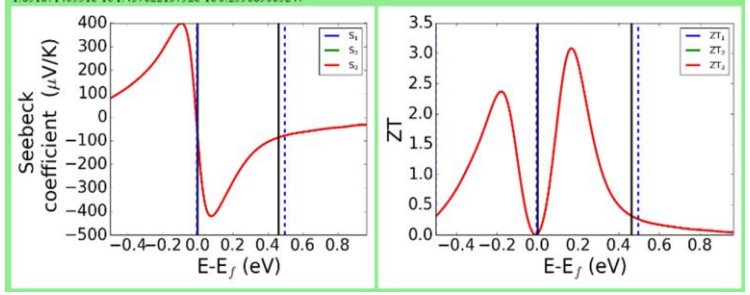
WARNING: Constant relaxation time approximation (10^{-14} s) and only electronic contribution to thermal conductivity were utilized for calculating ZT.

Electron mass tensor (m_e unit)

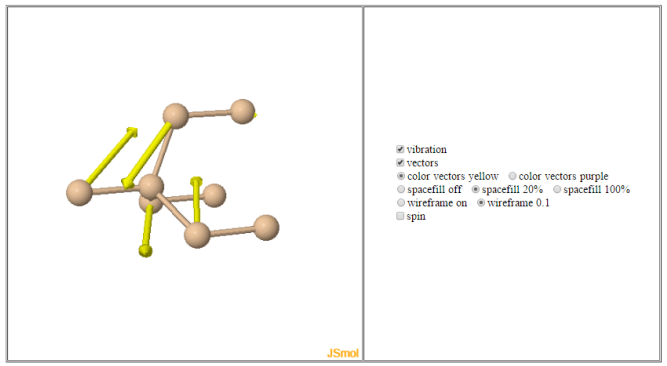
0.213343254384 7.30501044958e-17 1.81890909804e-16
7.30501044958e-17 0.213342672914 1.38823476056e-16
1.81890909804e-16 1.38823476056e-16 0.213342995953

Hole mass tensor (m_e unit)

0.259689400293 6.59511675992e-17 1.85187140551e-16
6.59511675992e-17 0.259688682339 1.43762213792e-16
1.85187140551e-16 1.43762213792e-16 0.259689065247



Right click on the atomic structure. Then select third option "model" and then select the frequency to be visualized.



Visualization of phonon modes

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 calcuation are also shown.

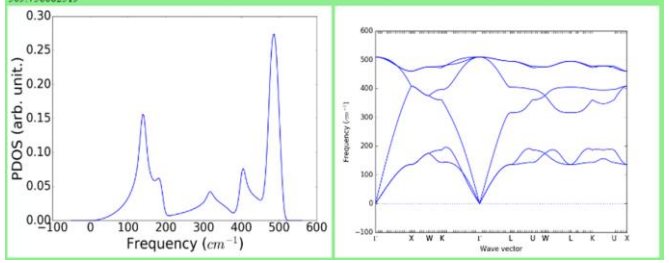
WARNING: Please note this may not be the exact phonon modes of the system as we did not test the cell-size dependence of phonons yet. At least 1.2 nm x1.2 nm x1.2 nm or more is needed for obtaining reliable phonon spectrum. For systems having primitive-cell phonon representation tables, I denotes infrared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

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})

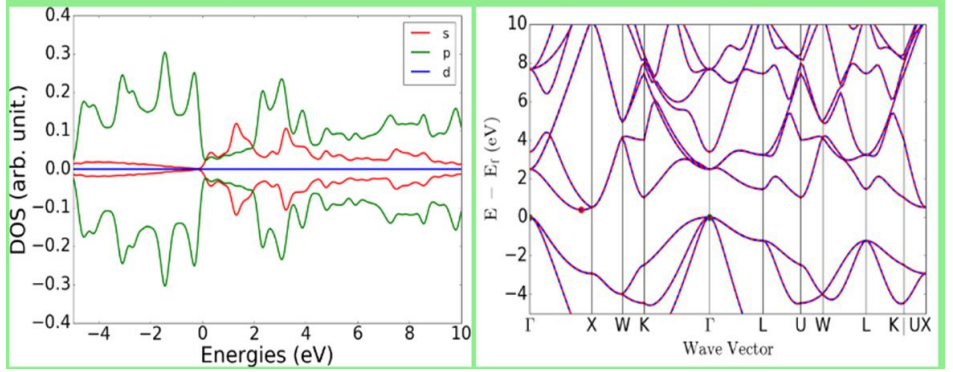
-0.0521466365
-0.0521466361
-0.0521466347
136.239760177
408.173817129
460.782147546
509.756682519

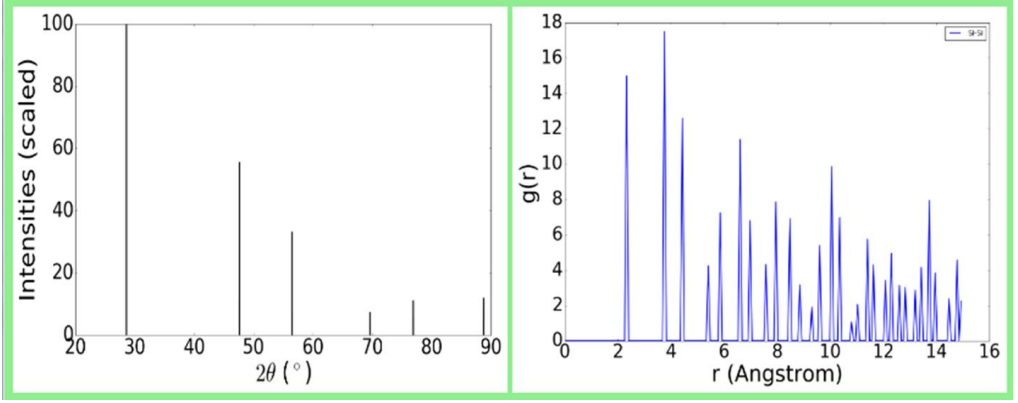


Electronic structure

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



Structural analysis

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