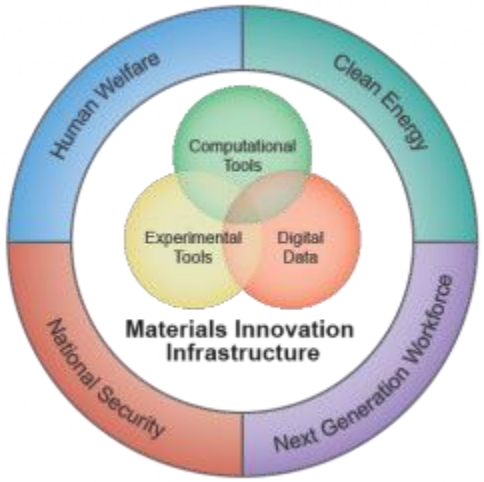

JARVIS

Computational Discovery of Two-Dimensional Materials, Evaluation of Force-Fields and Machine Learning

By

Kamal Choudhary

Northwestern University, May 19, 2017

NIST Materials Genome Initiative
Gateway to Materials Genome Information

Acknowledgments


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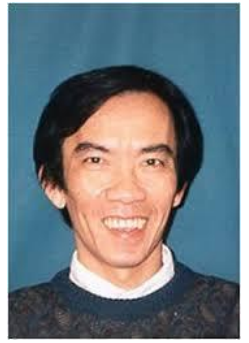

NIST

Others : Richard Hennig (UF), Susan Sinnott (PSU), Tao Liang (PSU), Kiran Mathew (LBNL), Kristin Persson (LBNL)
Computational resources: CTCMS, RARITAN, XSEDE, NERSC
Software packages: VASP, LAMMPS, Pymatgen, ASE, Phonopy, Magpie, Matminer, Flask

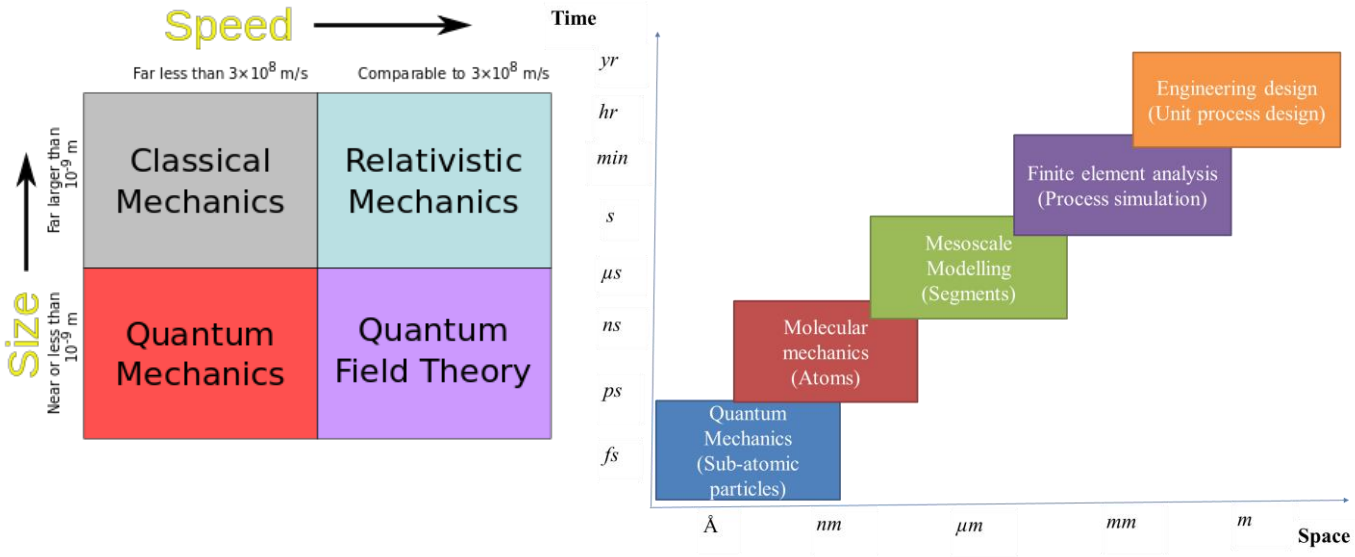
Outline

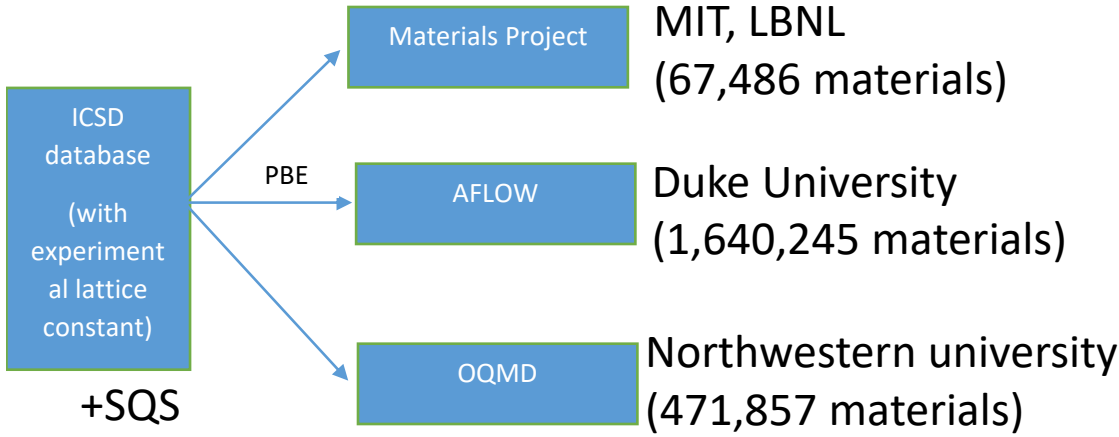
1. JARVIS-FF
   - Evaluation of elastic constants, convex hull
   - Defects, surfaces, phonons
2. JARVIS-DFT:
   - 2D or not 2D?
   - Properties
3. JARVIS-ML:
   - Generalized Material-descriptors/features (challenge?)
   - Neural-Network+classical physics based hybrid force-field
4. Conclusions

Email: kamal.choudhary@nist.gov

Few basics

- Materials Science is all about: Structure-Property-Performance relationship and minimization of free-energy
- Computationally: Structure = lattice constants (a,b,c), angles (alpha, beta, gamma) and basis vectors ([Si,0, 0,0],[Si,0.5,0.0,0.5],…..)
- To calculate property: classical physics (e.g. classical force-fields), quantum physics (e.g. density functional theory)
- MGI motivated current computational databases: Materials-project (MP), AFLOW, OQMD





Email: kamal.choudhary@nist.gov

Others: AIIDA, MaterialWeb, NREL-MatDB etc.

JARVIS-FF

1A Introduction to force-fields

1B Property evaluation: elastic constants, convex hull

1C Defects, surfaces, phonons

Email: kamal.choudhary@nist.gov

1A Intro Force-fields

- Coulomb potential $V(q_1(\vec{r}_1), q_2(\vec{r}_2)) = \frac{kq_1q_2}{|\vec{r}_2 - \vec{r}_1|}$ One parameter to fit/optimize
- Lennard-Jones potential $V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$ Repulsive and attractive terms, Two parameters to fit
- Morse-potential $V(r) = D_e(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)})$

These potentials lack angular information hence not able to capture elastic constants well

- Stilinger-Weber potential $V_{TOT} = \sum_{i,j}^{N} V_2(r_{ij}) + \sum_{i,j,k}^{N} V_3(r_{ij}, r_{ik}, \theta_{ijk})$ Uses angle but transferability problem
- EAM and MEAM potential $V_{TOT} = \sum_{i}^{N} F_i\left(\sum_{j} \rho(r_{ij})\right) + \frac{1}{2}\sum_{i,j}^{N} V_2(r_{ij})$ Uses electron density, for metallic systems
- Bond-order/Tersoff/Brenner $V_{ij}(r_{ij}) = V_{repulsive}(r_{ij}) + b_{ijk}V_{attractive}(r_{ij})$ Uses bond information, for covalent systems

These potentials lack charge information

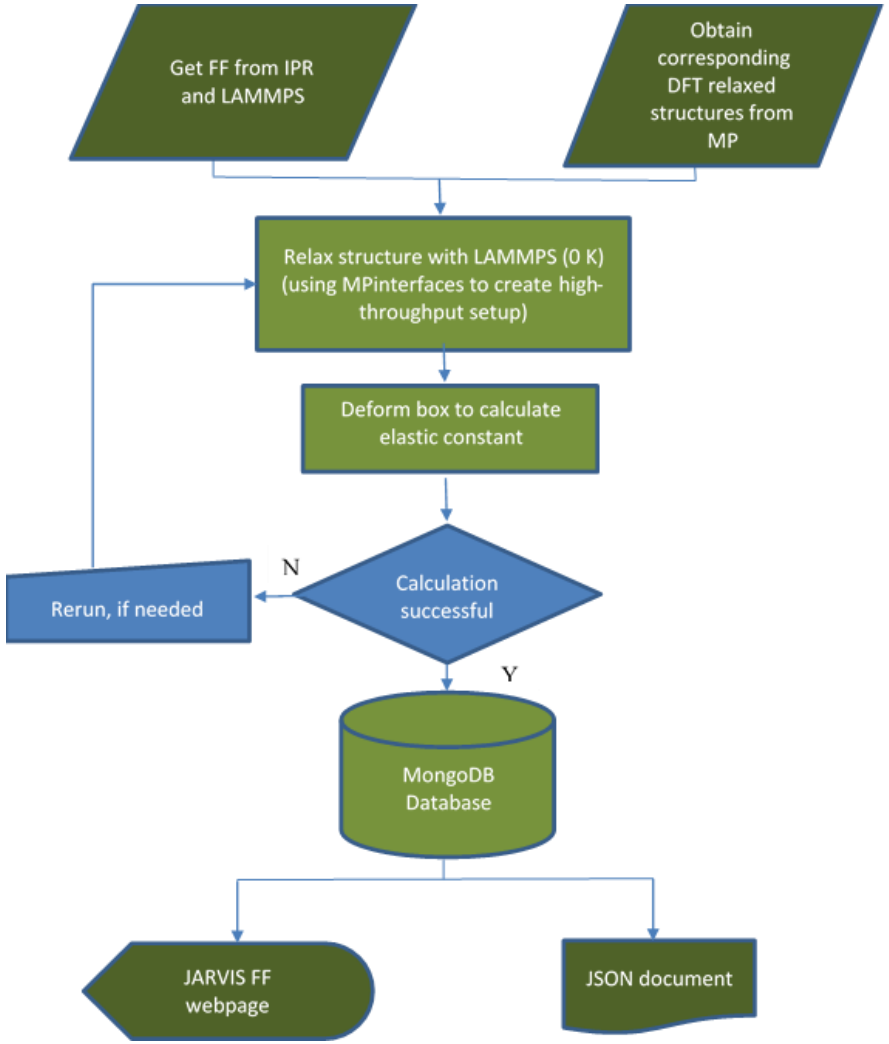
- Fixed charge potentials: Coulomb-Buckingham
- Other FFs: ReaxFF, COMB, AMBER, CHARMM, OPLS etc.

$$F_i = m_i a_i, \quad F_i = -\nabla_i V, \quad -\frac{dV}{dr_i} = m_i \frac{d^2 r_i}{dt^2}$$

Berni Alder

Email: kamal.choudhary@nist.gov

JARVIS-FF-workflow



- Force-fields obtained from NIST's interatomic potential repository and LAMMPS-potential folder (e.g. Mishin-Ni-Al-2009.alloy)
- DFT relaxed structures obtained from materials-project for corresponding system (say Ni-Al system: Al, Ni, Ni3Al, NiAl etc.)
- Convert the files from DFT format to LAMMPS format write corresponding input files from LAMMPS
- HT LAMMPS calculations

Email: kamal.choudhary@nist.gov

Public Webpage

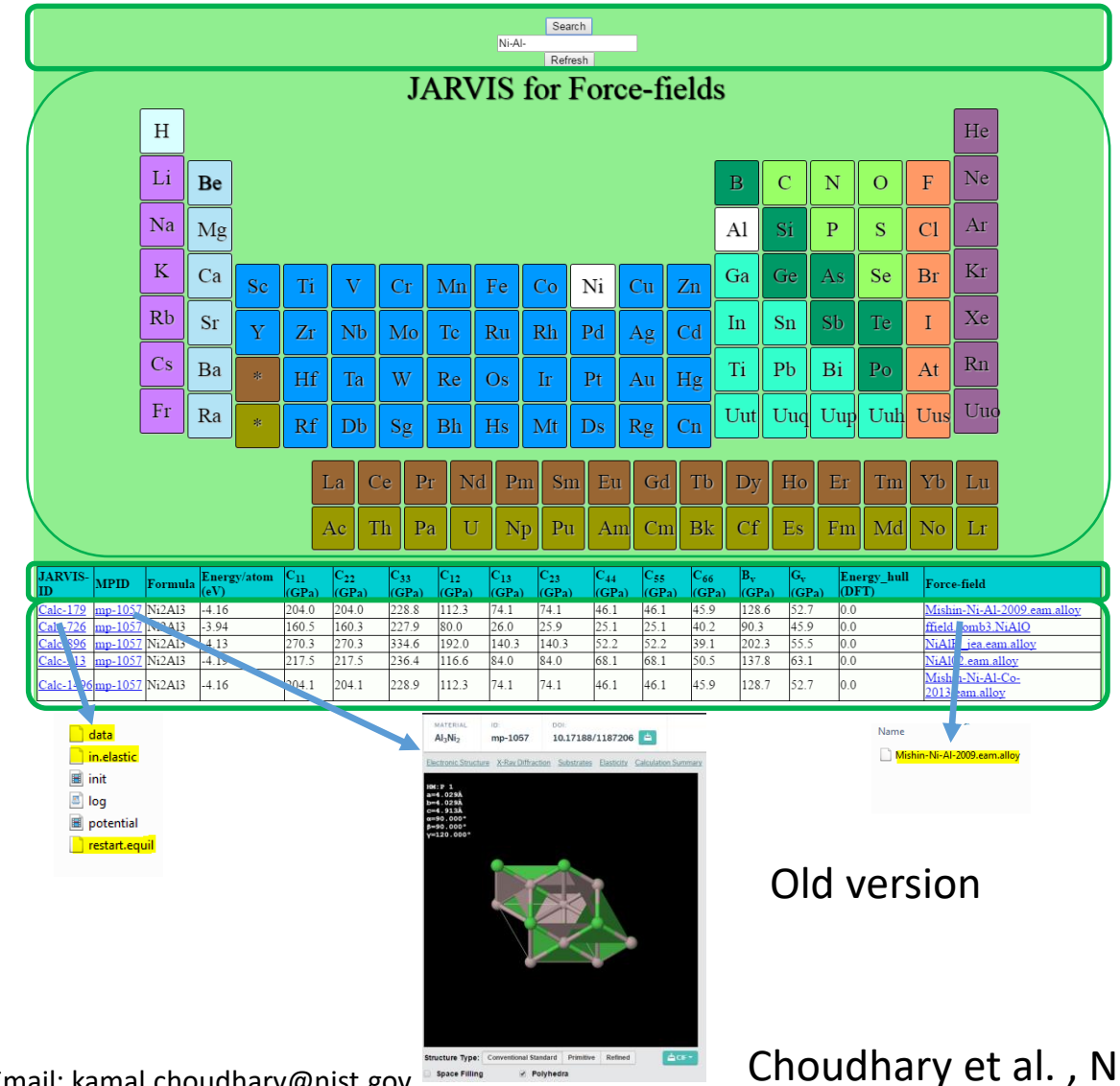
a)

b)

http://www.ctcms.nist.gov/~knc6/periodic.html
http://www.ctcms.nist.gov/~knc6/JLAMMPS.html

c)

d)



JARVIS-ID	MPID	Formula	Energy/atom (eV)	C_{11} (GPa)	C_{22} (GPa)	C_{33} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{23} (GPa)	C_{44} (GPa)	C_{55} (GPa)	C_{66} (GPa)	B_v (GPa)	G_v (GPa)	Energy_hull (DFT)	Force-field
Calc-179	mp-1057	Ni2Al3	-4.16	204.0	204.0	228.8	112.3	74.1	74.1	46.1	46.1	45.9	128.6	52.7	0.0	Mishin-Ni-Al-2009.eam.alloy
Calc-726	mp-1057	Ni2Al3	-3.94	160.5	160.3	227.9	80.0	26.0	25.9	25.1	25.1	40.2	90.3	45.9	0.0	ffield.comb3.NiAlO
Calc-896	mp-1057	Ni2Al3	-4.13	270.3	270.3	334.6	192.0	140.3	140.3	52.2	52.2	39.1	202.3	55.5	0.0	NiAlH_jea.eam.alloy
Calc-913	mp-1057	Ni2Al3	-4.13	217.5	217.5	236.4	116.6	84.0	84.0	68.1	68.1	50.5	137.8	63.1	0.0	NiAlO.eam.alloy
Calc-1296	mp-1057	Ni2Al3	-4.16	204.1	204.1	228.9	112.3	74.1	74.1	46.1	46.1	45.9	128.7	52.7	0.0	Mishin-Ni-Al-Co-2013.eam.alloy

Old version

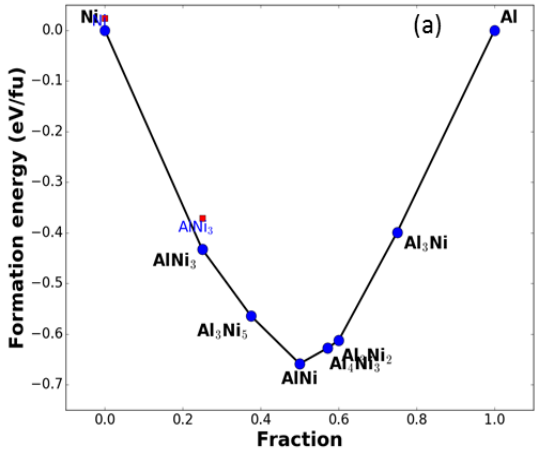
JARVIS-ID	Formula	Spacegroup	Energy/atom (eV)	C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{44} (GPa)	B_v (GPa)	G_v (GPa)	Force-field
JLMP-165	AlNi3	Pm-3m	-4.631478	238.2	166.4	166.4	130.2	190.3	92.5	Mishin-Ni-Al-2009.eam.alloy
JLMP-166	AlNi	Pm-3m	-4.510871	190.9	142.9	142.9	121.5	158.9	82.5	Mishin-Ni-Al-2009.eam.alloy
JLMP-167	Al3Ni5	Cmmm	-4.582119875	188.1	178.5	179.7	86.7	201.0	95.0	Mishin-Ni-Al-2009.eam.alloy
JLMP-168	Al3Ni	Pnma	-3.87520775	208.5	105.8	93.0	43.1	119.3	36.6	Mishin-Ni-Al-2009.eam.alloy
JLMP-169	Al4Ni3	Ia-3d	-4.26581160714	187.6	117.8	117.8	77.4	141.1	60.4	Mishin-Ni-Al-2009.eam.alloy
JLMP-170	AlNi3	Fm-3m	-4.59878825	197.3	180.7	180.7	138.9	186.2	86.7	Mishin-Ni-Al-2009.eam.alloy
JLMP-171	Al3Ni2	P-3m1	-4.1589292	204.0	112.3	74.1	46.1	128.6	52.7	Mishin-Ni-Al-2009.eam.alloy
JLMP-179	AlNi3	Pm-3m	-4.631478	238.2	166.4	166.4	130.2	190.3	92.5	Mishin-Ni-Al-Co-2013.eam.alloy
JLMP-180	AlNi	Pm-3m	-4.510871	190.8	142.9	142.9	121.5	158.9	82.5	Mishin-Ni-Al-Co-2013.eam.alloy
JLMP-181	Al3Ni5	Cmmm	-4.582119875	188.1	178.5	179.8	86.7	201.1	95.0	Mishin-Ni-Al-Co-2013.eam.alloy
JLMP-182	Al3Ni	Pnma	-3.87520775	208.5	105.8	93.0	43.1	119.3	36.6	Mishin-Ni-Al-Co-2013.eam.alloy
JLMP-183	Al4Ni3	Ia-3d	-4.26581160714	187.6	117.8	117.8	77.4	141.1	60.4	Mishin-Ni-Al-Co-2013.eam.alloy
JLMP-184	AlNi3	Fm-3m	-4.59878825	197.3	180.7	180.7	138.9	186.2	86.7	Mishin-Ni-Al-Co-2013.eam.alloy
JLMP-185	Al3Ni2	P-3m1	-4.1589292	204.1	112.3	74.1	46.1	128.7	52.7	Mishin-Ni-Al-Co-2013.eam.alloy
JLMP-209	AlNi3	Pm-3m	-4.631478	238.2	166.4	166.4	130.2	190.3	92.5	Mishin_updated-Ni-Al-Co-2013.eam.alloy
JLMP-210	AlNi	Pm-3m	-4.510871	190.8	142.9	142.9	121.5	158.9	82.5	Mishin_updated-Ni-Al-Co-2013.eam.alloy

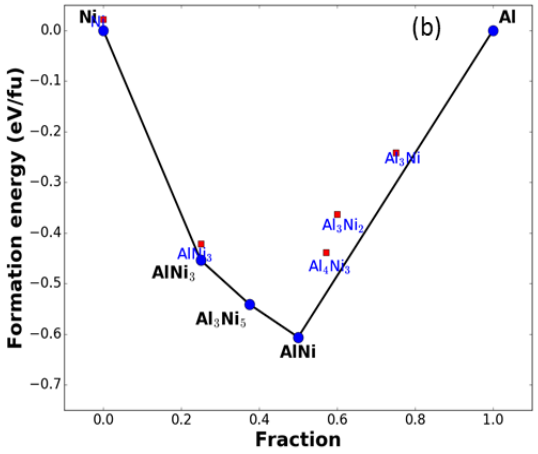
Development version

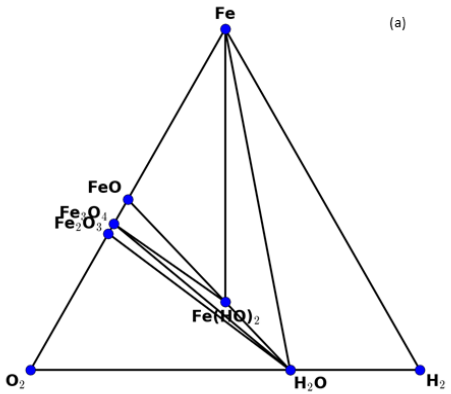
Email: kamal.choudhary@nist.gov

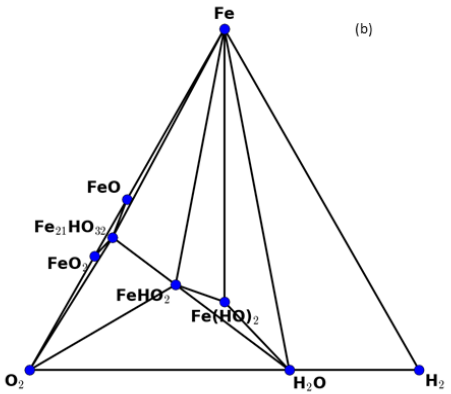
Choudhary et al. , Nature:Scientific Data 4, 160125 (2017)

1B Convex-hull plot







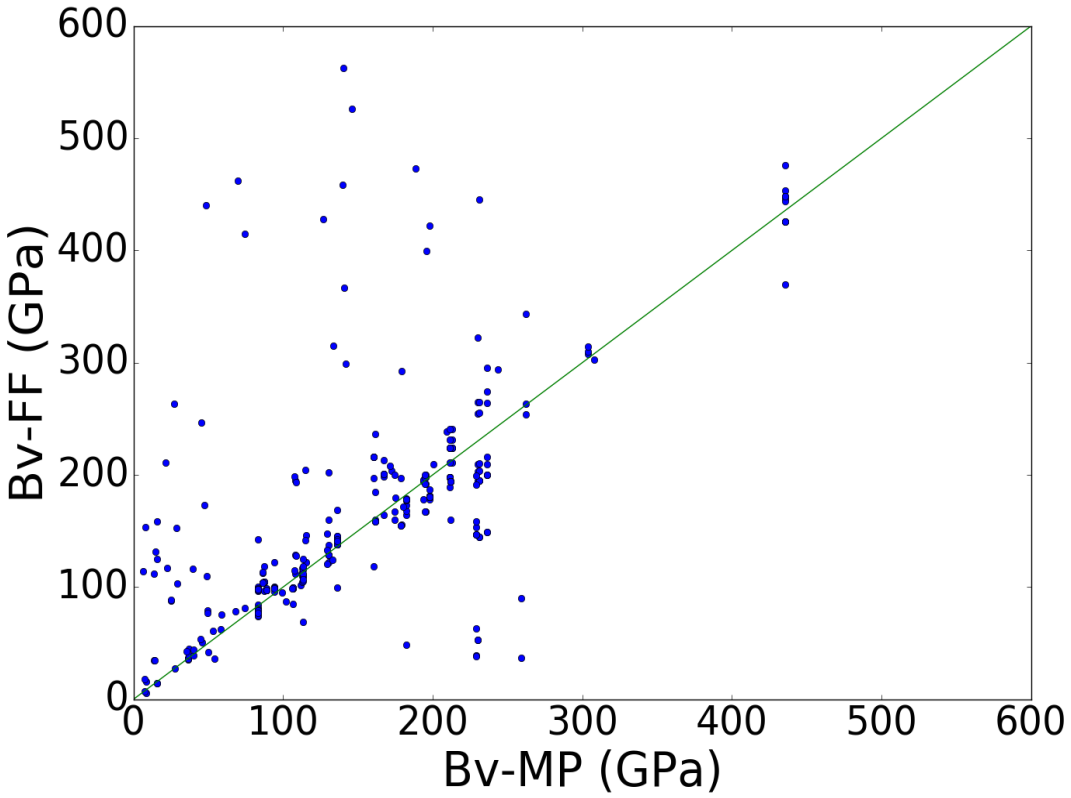


- Comparison of DFT convex-hull plot with LAMMPS
- Some points shown unstable for FF, because they are not fit to it !

Choudhary et al., Nature:Scientific Data 4, 160125 (2017)
Choudhary et al., Computational Materials Science 113, 80 (2016)

Email: kamal.choudhary@nist.gov

1B Bulk modulus



- Comparison of DFT bulk modulus with LAMMPS, ~500 points in common
- Some FFs are not fit for elastic properties

Choudhary et al, Nature:Scientific Data 4, 160125 (2017)

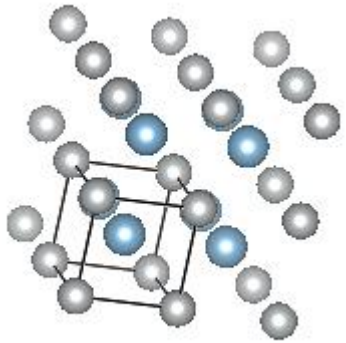
Email: kamal.choudhary@nist.gov

1C Vacancy formation energies

Vacancy-formation energy (eV)

Vacancy formation energies were calculated by deleting the symmterically 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	1	2.027
Ni	1	2.845



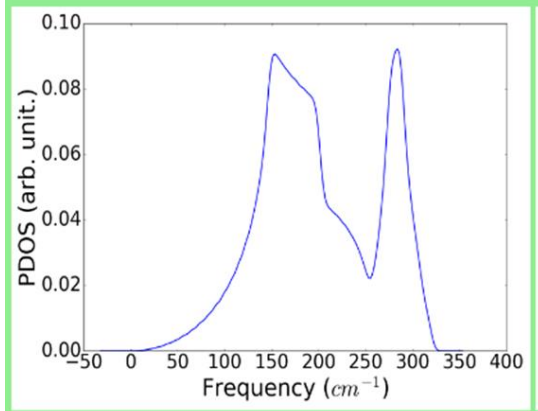
- Real materials are VERY defective !
- Vacancy structures based on unique Wyckoff positions
- Delete symmetrically distinct sites only

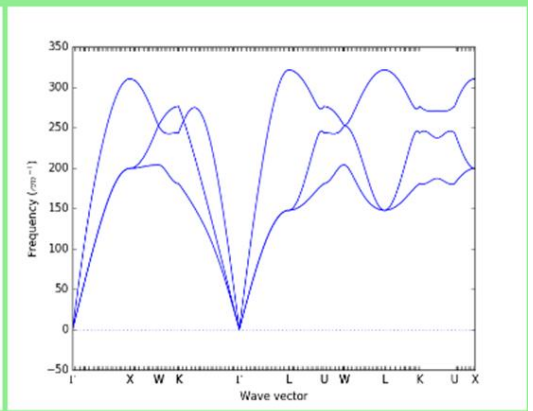
Email: kamal.choudhary@nist.gov

1C Phonons

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 deofrmed 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

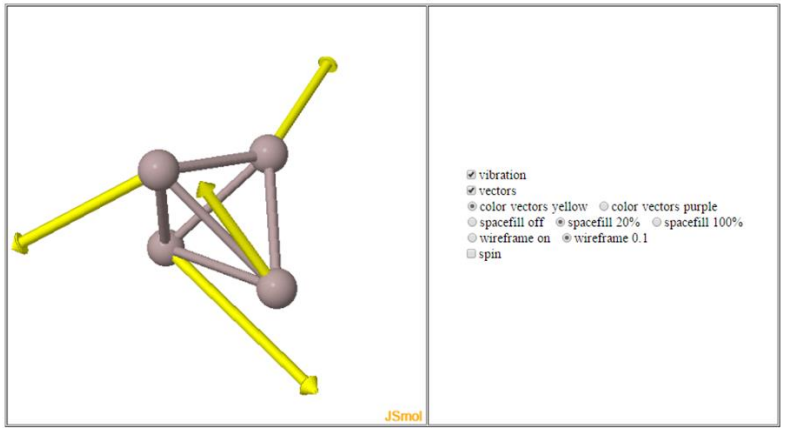
-1.3684e-05 T1u I

All phonon mode at Gamma point (cm^{-1})

-1.3874e-05
-1.2885e-05
-1.03024e-05
199.579415818
310.632537509

Reference

mp-134



$$\Phi = \Phi_0 + \sum_{lk} \Phi_\alpha(lk) u_\alpha(lk) + \frac{1}{2} \sum_{ll'kk'} \Phi_{\alpha\beta}(lk, l'k') u_\alpha(lk) u_\beta(l'k') + \dots$$

$$\Phi_{\alpha\beta}(lk, l'k') = -\frac{\partial F_\beta(l'k')}{\partial u_\alpha(lk)} = \frac{\partial^2 \Phi}{\partial u_\alpha(lk) \partial u_\beta(l'k')}.$$

$$D^{kk'}_{\alpha\beta}(\mathbf{q}) = \frac{1}{\sqrt{M_k M_{k'}}} \sum_{l'} \Phi_{\alpha\beta}(0k, l'k') e^{i\mathbf{q}[\mathbf{r}(l'k') - \mathbf{r}(0k)]}$$

$$\sum_{\beta k'} D^{kk'}_{\alpha\beta}(\mathbf{q}) e^{\beta k'}_{\mathbf{q}j} = \omega^2_{\mathbf{q}j} e^{\alpha k}_{\mathbf{q}j}$$

Email: kamal.choudhary@nist.gov

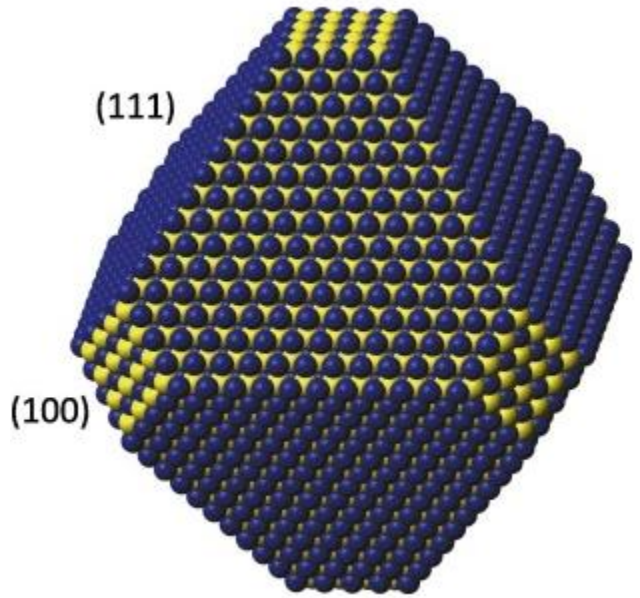
http://wiredspace.wits.ac.za/bitstream/handle/10539/21022/Dongho_Moise_704598_PhD_Thesis.pdf?sequence=1&isAllowed=y

1C Surface energies

Surface energy (J/m2)

Surface energies were calculated for symmterically distinct crystal surfaces obtained with Pymatgen. In the table, (hkl) indices and surface enegies are given. For surface-structure energetics, constant volume ensemble was used. We impose the slab thickness to be at least 2 nm and vaccum 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
(1 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
(2 2 1)	1.058



Wulff construction: Used in predicting equilibrium shape of materials

Mathew et al., Computational Materials Science, 122 183 (2016

Email: kamal.choudhary@nist.gov

Summary Part-1

- New website for FF calculation data
- Enable user to select FF before doing any calculations
- Can be complement to DFT where computational cost is too high, such as phonons, defects, grain boundaries etc.
- Genetic algorithm based evaluation, melting point, thermal expansion coefficient, thermal conductivity, Grüneisen parameter calculations on the way
- Outreach: thousands of website hits in few months, JARVIS-FF listed as a post-processing tools for LAMMPS

Email: kamal.choudhary@nist.gov

PART 2 JARVIS-DFT

2A Introduction to Density functional theory

2B 2D Materials

- Applications: Sub-micron electronics, Flexible and tunable electronics, photo-voltaics, energy-storage

Email: kamal.choudhary@nist.gov

2A Density Functional Theory

Second derivative wrt X

Schrodinger Wave-function

$$\frac{\partial^2\psi}{\partial x^2}+\frac{8\pi^2 m}{h^2}(E-V)\psi=0$$

Position Energy Potential Energy

- Classical Newton's laws not applicable for electrons (**very fast, very tiny**);
- Schrödinger equation: mathematical equation that describes the evolution over time of a physical system in which quantum effects, such as **wave–particle duality**, are significant (such as electrons)
- Schrödinger equation of a **fictitious system** (the "Kohn–Sham system") of **non-interacting particles** (typically electrons) that generate the **same density** as any given system of interacting particles
- Uses **density** (scalar) vs **wavefunction** (vector) quantity

Exchange-correlation

$$H\psi=E\psi \qquad \left[-\frac{\hbar^2}{2m}\nabla^2+V_{Eff}(r)\right]\psi_i(r)=E_i(r)\psi_i(r) \qquad V_{Eff}=T+V_{Ne}+V_{ee}+V_{XC}$$

Walter Kohn

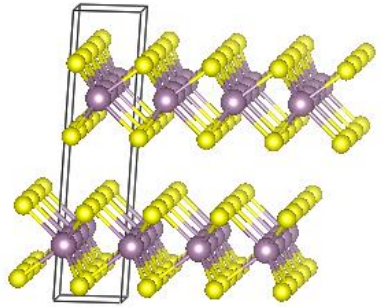
- **Different functionals: LDA, GGA (PBE, PW91), HSE06 etc.**
- **LDA**: developed for homogenous systems (Thomas-Fermi model), such as metals
- **GGA**: uses density gradient information on top of GGA
- **vdW-DF2**: uses exchange from GGA, correlation from LDA, quantum-Monte-Carlo based non-local corrections, **optB88** used here mainly

Hohenberg, Pierre; Walter Kohn (**1964**). "Inhomogeneous electron gas". *Physical Review*. **136** (3B): B864–B871

https://en.wikipedia.org/wiki/Classical_mechanics
http://www.psi-k.org/Update3.shtml
http://www.physlink.com/Education/AskExperts/ae329.cfm

Email: kamal.choudhary@nist.gov

2B Two-dimensional materials

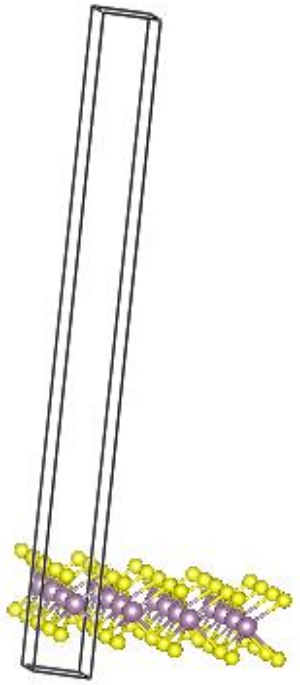


- Vander-Waal bonding in z-direction, covalent bonding in x, y-directions, e.g. Graphene,MoS_2

DIMENSIONALITY ==PERIODICITY

- Easily exfoliated, scotch-tape type, potential candidate for sub-nanometer technology, Si-replacement, flexible electronics, and other applications
- **For DFT calculation on 2D materials**: position of atoms (r) obtained from XRD and other experiments, ICSD database and other DFT databases
- DFT databases (**Materials Project, AFLOW, OQMD**) took structures from ICSD and used PBE functionals consistently for all structures, JARVIS-DFT took from them
- **Catch**: PBE functionals overestimate lattice constants (the r's in PBE-DFT are not correct)
- **JARVIS-DFT**: Using REST API at Materials-project got all the crystal structures with ICSD and PBE data and calculated relative error

$$\delta = \frac{|l_{PBE} - l_{ICSD}|}{l_{ICSD}}$$

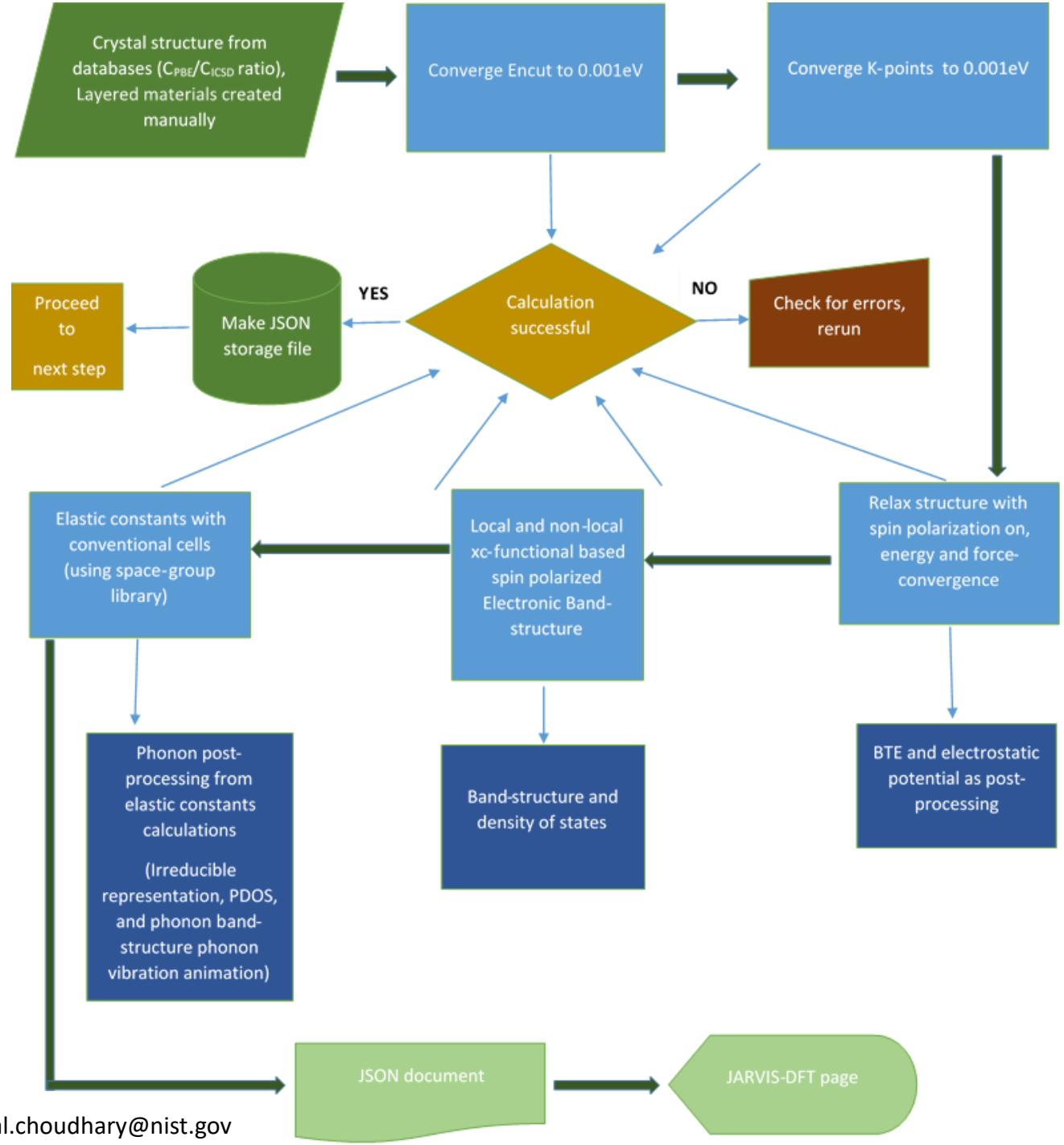


- If the error is more than **5%,** we predict them to be 2D materials; at least **1356 such materials** Found, recalculate with better optB88 functionals, tight DFT convergence

http://ammcttwtht.tumblr.com/post/101405895438/a-miracle-material-can-take-the-world-to-the

Email: kamal.choudhary@nist.gov

JARVIS-DFT workflow



- Written in python language
- Separate calculation for mono-layer and bulk materials
- Mono-layer created by adding additional vacuum (20 Angstrom) in z-direction
- c-lattice constant not-optimized for mono-layer (custom compilation of VASP)
- Example:

```
bulk@mp_48
   1.00000000000000
     1.2325005105744926   -2.1347529556398626    0.0000000000000000
     1.2325005105744926    2.1347529556398626    0.0000000000000000
     0.0000000000000000    0.0000000000000000    6.6962686124617425
   C
     4
Direct
  0.0000000000000000  0.0000000000000000  0.2500000000000000
  0.0000000000000000  0.0000000000000000  0.7500000000000000
  0.3333330000000032  0.6666669999999968  0.2500000000000000
  0.6666669999999968  0.3333330000000032  0.7500000000000000
```

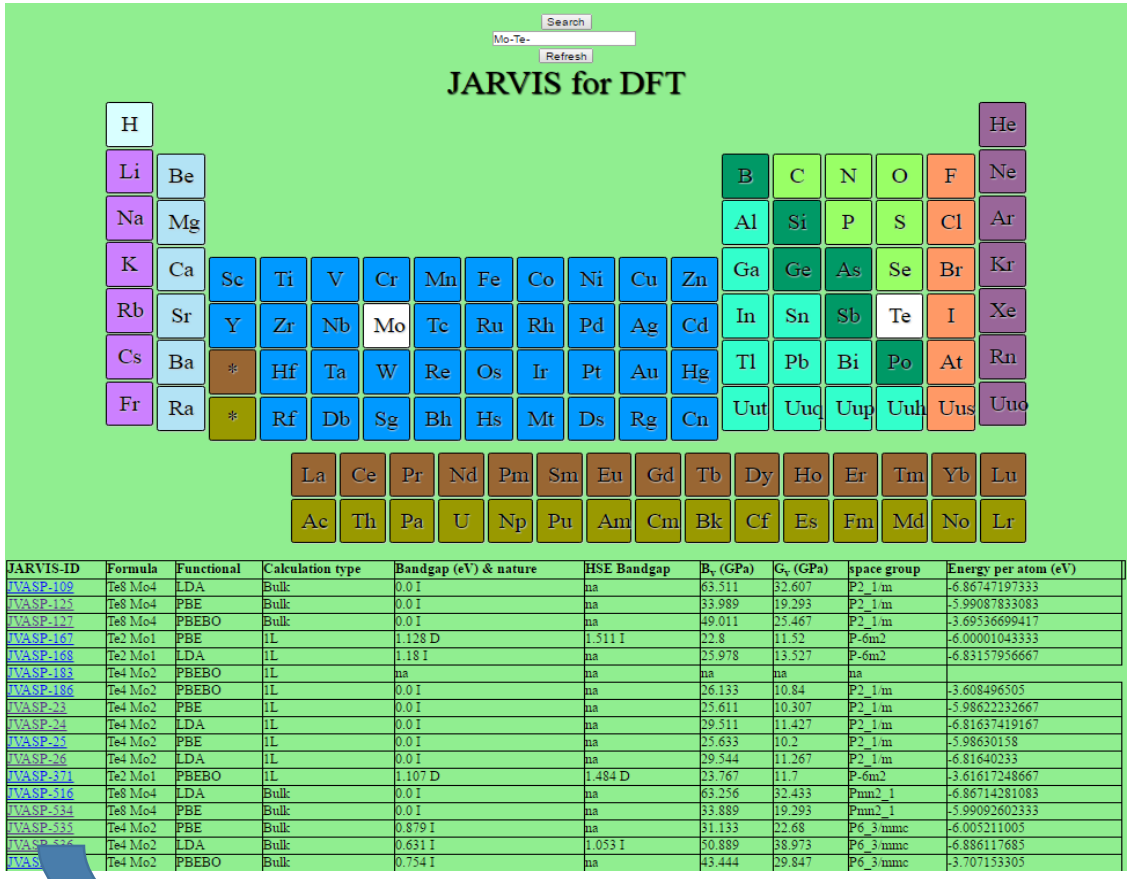
```
Surf-mp-48
   1.00000000000000
     1.2320971008984494   -2.1340542301747005    0.0000000000000000
     1.2320971008984494    2.1340542301747005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.8030730000000013
   C
     2
Direct
  0.0000000000000000  0.0000000000000000  0.0633300000000006
  0.3333330000000032  0.6666669999999968  0.0633300000000006
```


Email: kamal.choudhary@nist.gov

Webpage

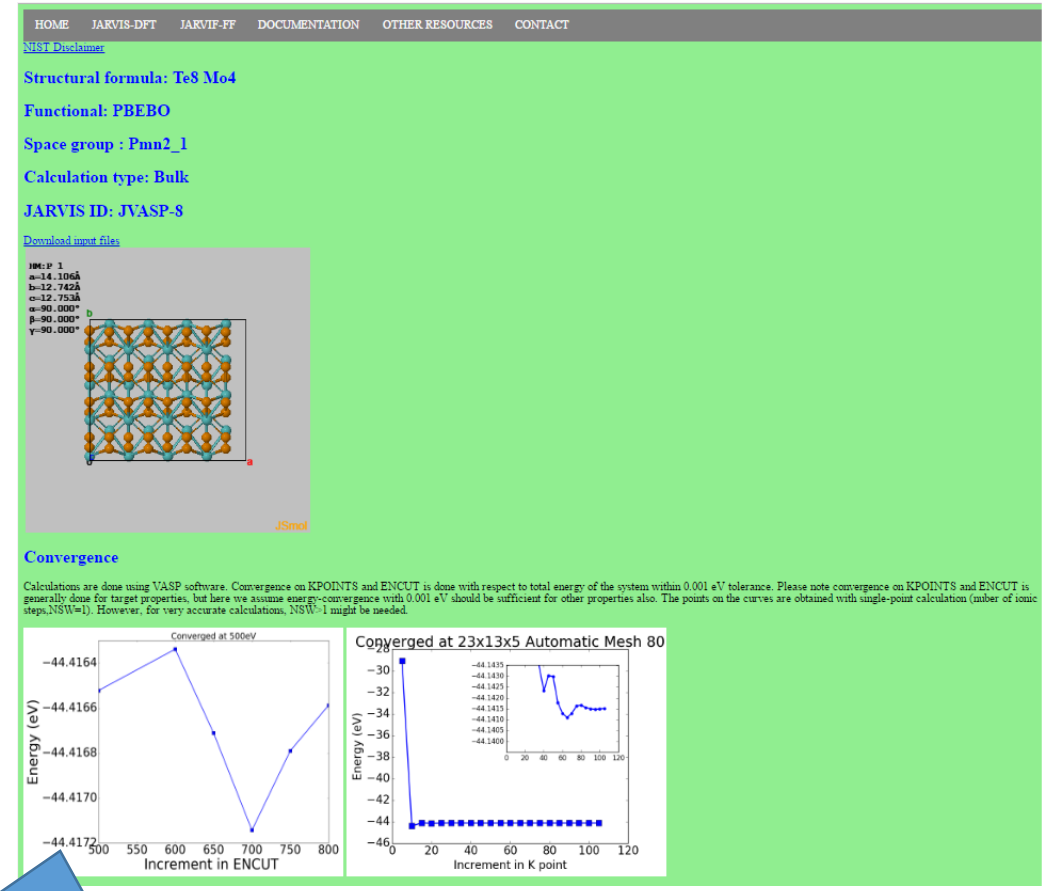
http://www.ctcms.nist.gov/~knc6/JVASP.html

- Click on elements, click search, click JARVIS-ID



JARVIS-ID	Formula	Functional	Calculation type	Bandgap (eV) & nature	HSE Bandgap	B_T (GPa)	G_V (GPa)	space group	Energy per atom (eV)
JVASP-109	Te8 Mo4	LDA	Bulk	0.0 I	na	63.511	32.607	P2_1/m	-6.86747197333
JVASP-125	Te8 Mo4	PBE	Bulk	0.0 I	na	33.989	19.293	P2_1/m	-5.99087833083
JVASP-127	Te8 Mo4	PBEBO	Bulk	0.0 I	na	49.011	25.467	P2_1/m	-3.69536699417
JVASP-167	Te2 Mo1	PBE	1L	1.128 D	1.511 I	22.8	11.52	P-6m2	-6.00001043333
JVASP-168	Te2 Mo1	LDA	1L	1.18 I	na	25.978	13.527	P-6m2	-6.83157956667
JVASP-183	Te4 Mo2	PBEBO	1L	na	na	na	na	na	
JVASP-186	Te4 Mo2	PBEBO	1L	0.0 I	na	26.133	10.84	P2_1/m	-3.608496505
JVASP-23	Te4 Mo2	PBE	1L	0.0 I	na	25.611	10.307	P2_1/m	-5.98622232667
JVASP-24	Te4 Mo2	LDA	1L	0.0 I	na	29.511	11.427	P2_1/m	-6.81637419167
JVASP-25	Te4 Mo2	PBE	1L	0.0 I	na	25.633	10.2	P2_1/m	-5.98630158
JVASP-26	Te4 Mo2	LDA	1L	0.0 I	na	29.544	11.267	P2_1/m	-6.81640233
JVASP-371	Te2 Mo1	PBEBO	1L	1.107 D	1.484 D	23.767	11.7	P-6m2	-3.61617248667
JVASP-516	Te8 Mo4	LDA	Bulk	0.0 I	na	63.256	32.433	Pmn2_1	-6.86714281083
JVASP-534	Te8 Mo4	PBE	Bulk	0.0 I	na	33.889	19.293	Pmn2_1	-5.99092602333
JVASP-535	Te4 Mo2	PBE	Bulk	0.879 I	na	31.133	22.68	P6_3/mmc	-6.005211005
JVASP-536	Te4 Mo2	LDA	Bulk	0.631 I	1.053 I	50.889	38.973	P6_3/mmc	-6.886117685
JVASP-537	Te4 Mo2	PBEBO	Bulk	0.754 I	na	43.444	29.847	P6_3/mmc	-3.707153305

- Kpoint, Energy cut-off and force convergence (N/A in other DFT databases, but very important!)
- Both bulk and single-layer materials available
- **Makes ~5 times slower, but much reliable**



- >1280 hits in <6months
- Soon will be part of Citrine database

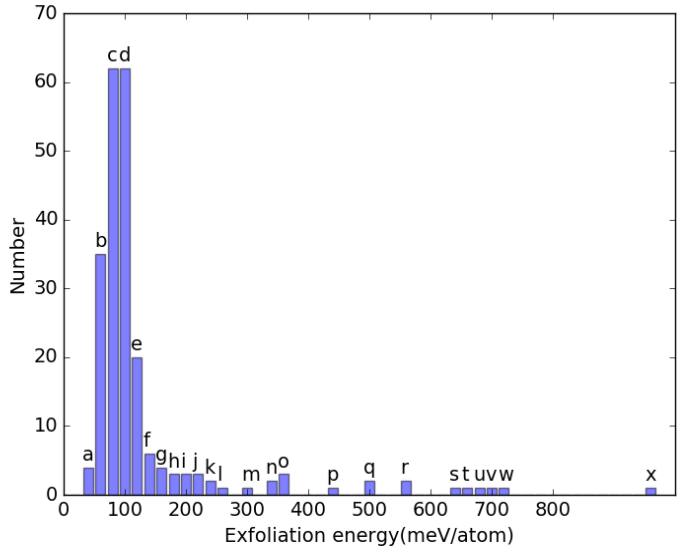
Read WARNINGS!

Email: kamal.choudhary@nist.gov

Exfoliation energy calculations

- Exfoliation energy:

$$E_f = \frac{E_{1L}}{N_{1L}} - \frac{E_{bulk}}{N_{bulk}}$$



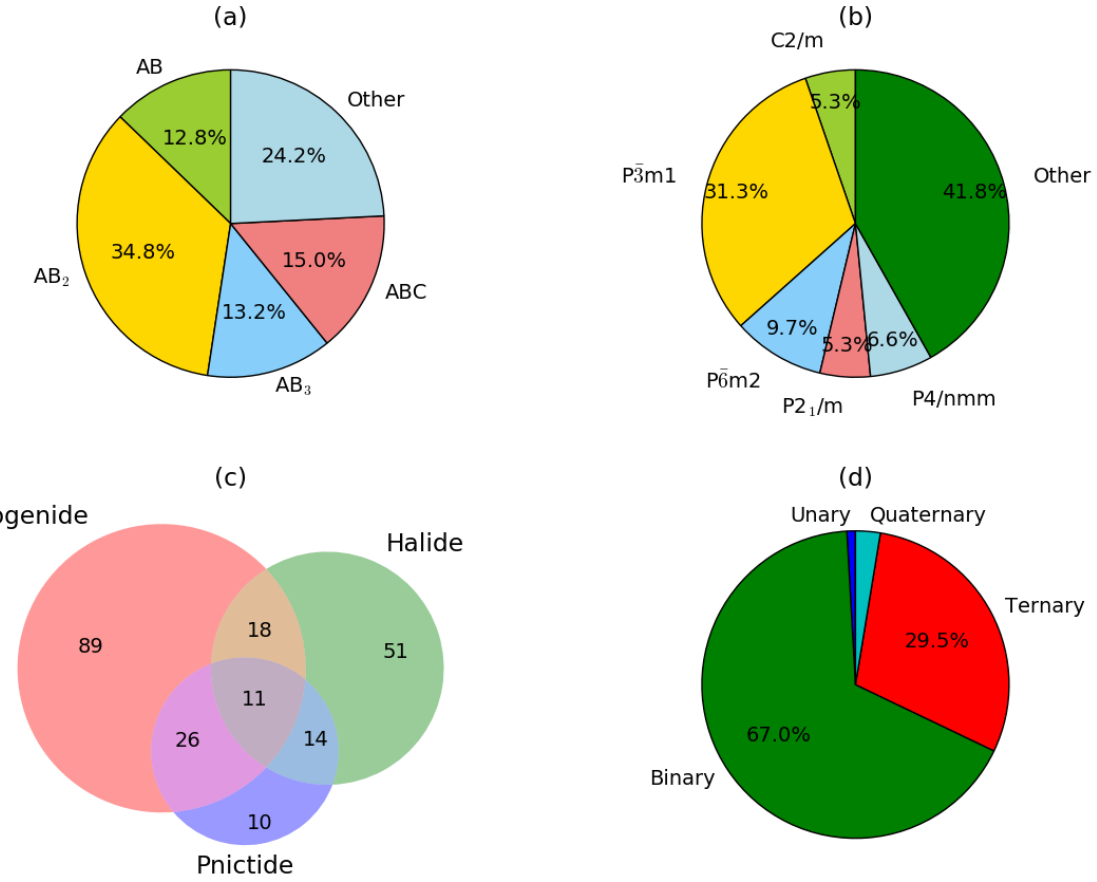
- 1012 bulk, 430 Single layer, 371 common, calculations still running (thousands of processors needed)

Choudhary et al., (Submitted)

	Energy range (meV)	Materials
a)	0-40	$TiNCl$, SiH_4, $HfBrN$, $Mg(AlSe_2)_2$
b)	40-60	$GaSe$, CrS_2, ZrS_3, NiO_2, GaS, $ZrSe_3$, $NdTe_3$, US_3, TiS_3, $PrIO$, $DySI$, Sc_2CCl_2, $ThIN$, $TiBrN$, $InClO$, $LuSBr$, $SrHI$, $BiIO$, $BiBrO$, $KMnP$, $TiIN$, Sc_2NCl_2, $TlSbO_3$, $ZrCl$, $SmTe_3$, $PrTe_3$, As_2O_3, Nb_2CS_2, $RbMnAs$, SiH, Bi_2TeI, $ScCl$, $TbBr$, $Ge(BiTe2)_2$, GaS
c)	60-80	WSe_2, WS_2, MoS_2, C, SnO_2, PtO_2, $CdBr_2$, $ReSe_2$, $CrSe$, $MgCl_2$, $CoBr_2$, $ZrCl_2$, $MgBr_2$, TcS_2, $FeCl_2$, $MnCl_2$, $MnBr_2$, $InSe$, $CrBr_3$, VCl_3, USe_3, $IrCl_3$, $ScCl_3$, $RhCl_3$, TaI_2O, $DySBr$, $ErSeI$, $ErSCl$, $BiClO$, $OsCl_2O$, $CdCl_2$, BN, $Nb(SCl)_2$, Bi_2Te_2S, $ThBrN$, $HfCl_4$, Bi_2Te_2Se, $MgPSe_3$, $CdPS_3$, $ScPS_4$, $PPdS$, $TmAg(PSe_3)_2$, $ScAg(PSe_3)_2$, $ErAg(PSe_3)_2$, $ScAg(PS_3)_2$, Nb_3Cl_8, Nb_3TeCl_7, $InAg(PSe_3)_2$, Hf_3Te_2, $SNCl$, Sr_3Si_2, $TiCl_2$, $HfFeCl_6$, $GaTe$, CS_2, $Nb(SeCl)_2$, $CrCl_3$, BiI, $TiBr_2$, $GaAg(PSe_3)_2$, $CdPS_3$, TiS_2
d)	80-100	NbS_2, $MoSe_2$, $NbSe_2$, WTe_2, $MoTe_2$, VSe_2, ZrS_2, HfS_2, $HfSe_2$, MoS_2, PtO_2, PtS_2, SnS_2, $SnSe_2$, TiO_2, TiS_2, $TiSe_2$, $ZrSe_2$, TaS_2, $SiTe_2$, $TaSe_2$, VS_2, $TaSe_2$, MgI_2, SbI_3, PbI_2, GeI_2, SiS_2, MnI_2, CaI_2, $RhBr_3$, BiI_3, $MoBr_3$, $RuBr_3$, PCl_3, AuI, BPS_4, $IrBr_3$, $Re(AgCl_3)_2$, $AlPS_4$, $AlSiTe_3$, $PPdSe$, $CrSiTe_3$, Nb_3TeI_7, NdI_2, Al_2Te_3, S_5N_6, $AlTeI_7$, $AlSeBr_7$, CdI_2, PSe, Ta_3TeI_7, TmI_2, $SbBr_3$, P_4S_5
e)	100-120	$HfTe_2$, $PtSe_2$, $TiTe_2$, WO_2, SnO, BCl_3, Te_2Br, Te_2I, PBr_3, TiI_3, $BiTeCl$, $BiTeI$, $TlPt_2S_3$, $AlBr_3$, $BiSBr$, CaN, Mn_2Bi, HgI_2, $SrThBr_6$, P
f)	120-140	BBr_3, AlI_3, $TlTe_3Pt_2$, $SbSBr$, $TlPd_2Se_3$, P_2Se_5
g)	140-160	PdS_2, Te_2Pt, BI_3, $Ta(ICl)_2$
h)	160-180	$PdSe_2$, $NiTe_2$, NbI_5
i)	180-200	ZrS, PI_3, $BaBrCl$
j)	200-220	Te_2Pd, Te_2Ir, $BiSe_2$
k)	220-240	$SbSeI$, $BiSI$
l)	240-260	Bi_2Te_3
m)	260-300	VS_2
n)	300-340	$CaSn$, $KAuSe$
o)	340-360	$KAuS$, $RbAuS$, $RbAuSe$
p)	360-440	Sc_2C
q)	440-500	GaN, $TiSe_2$
r)	500-560	Sr_2H_3, Ca_2H_3
s)	560-640	AlN
t)	640-660	$TiTe_2$
u)	660-680	$CrSe_2$
v)	680-700	$ZrTe_2$
w)	700-720	$CoAs_2$
x)	720-960	Ti_2O

Email: kamal.choudhary@nist.gov

Classification of database

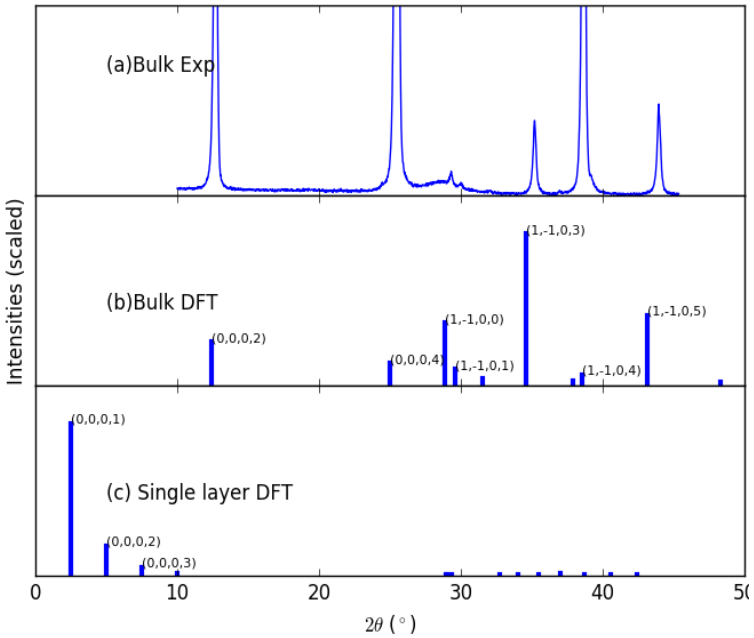


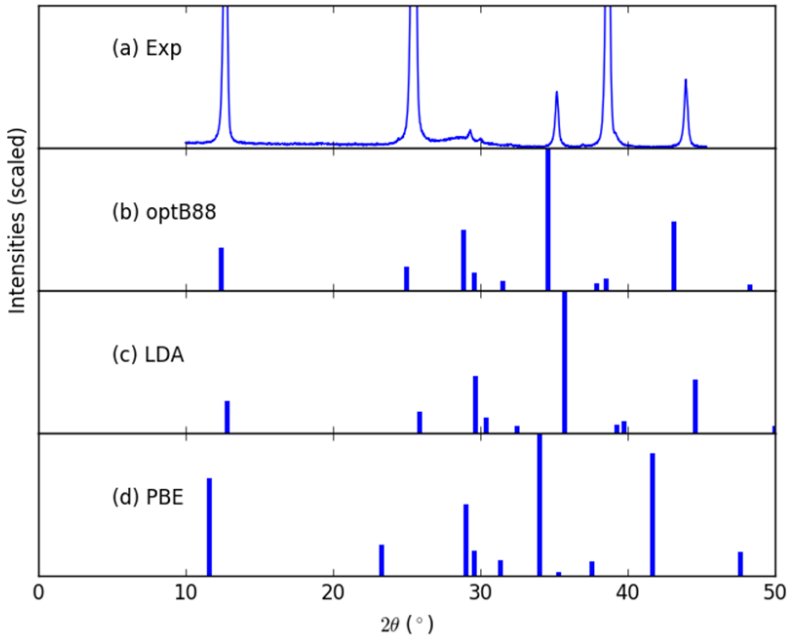
- 2D materials are not just AB2
- More than *2H* ($P\bar{6}m2$) and *1T* ($P\bar{3}m1$) prototype
- Venn diagram
- Majority of 2D materials are binary

Choudhary et al., (Submitted)

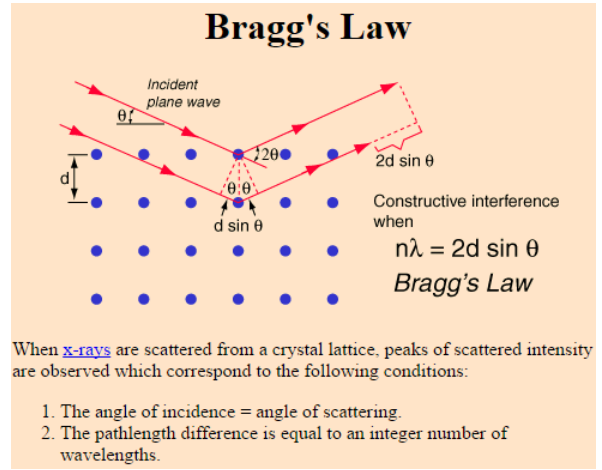
Email: kamal.choudhary@nist.gov

Computational X-Ray diffraction





- Computational X-ray diffraction:



- Experimental data from Irina Kalish ($MoTe_2$-2H)
- Computational XRD implemented in pymatgen
- Excellent agreement of optB88 and experiments
- PBE gives erroneous peaks
- Single-layer XRD also available

Choudhary et al., (Submitted)

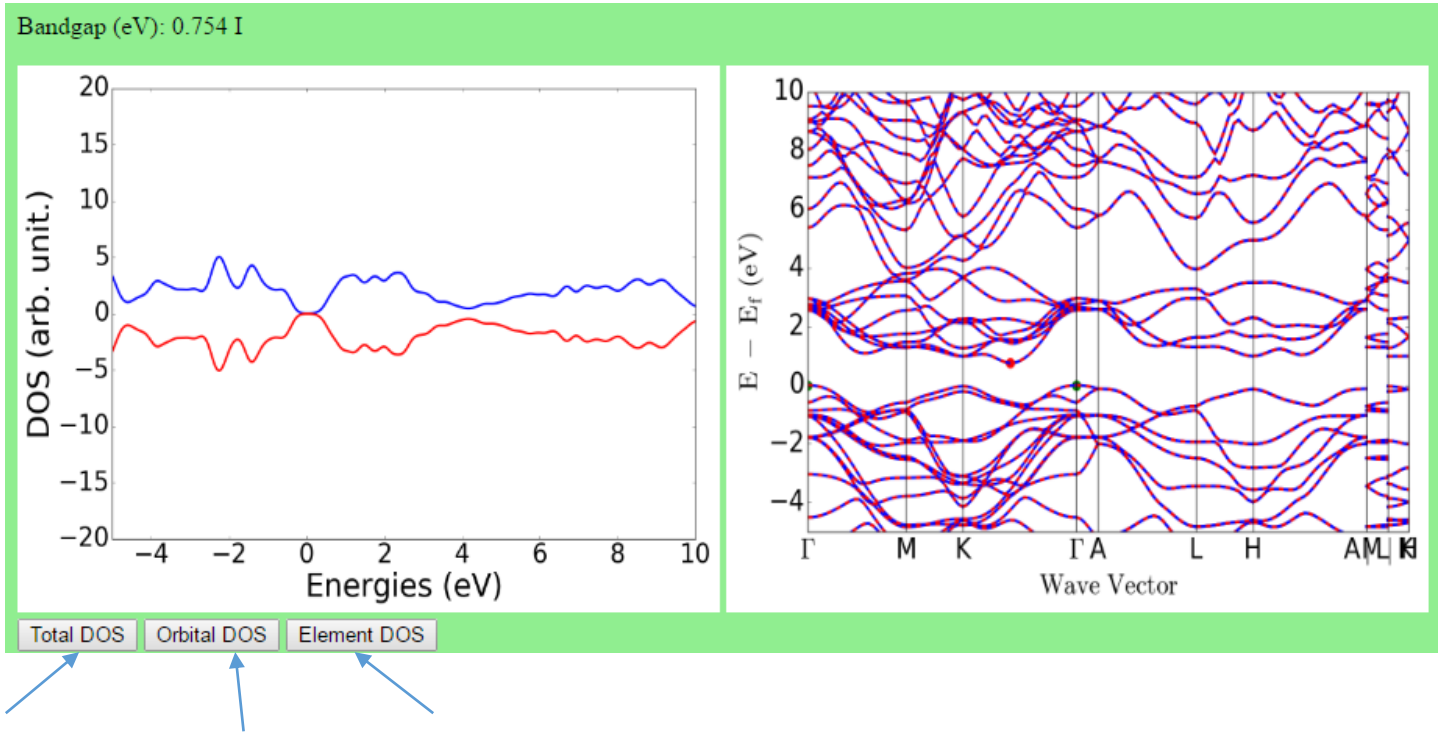
Email: kamal.choudhary@nist.gov

Read WARNINGS!

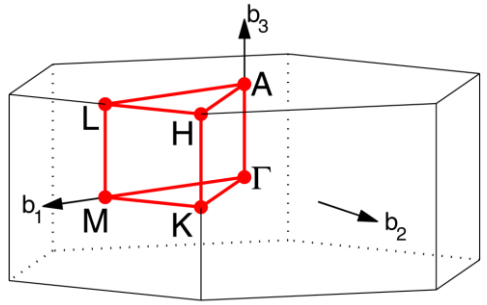
http://faculty.gvsu.edu/majumdak/public_html/OnlineMaterials/XRay.pdf
http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/bragg.html

Computational band-structure

- Density of states and Band-structures:



- optB88 bandgaps
- Few LDA, PBE and **HSE06 bandgaps**



HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Brillouin zone for hexagonal system

- DOS can be used to approximately calculate magnetic property such as **Orbital magnetic moment**

Email: kamal.choudhary@nist.gov

Read WARNINGS!

Elastic constants, Γ-point phonons

Elastic Tensor C_{ij} GPa

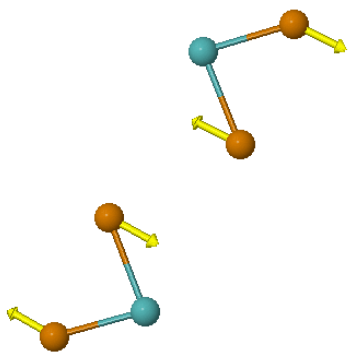
119.5	32.8	11.3	0.0	0.0	0.0
32.8	119.5	11.3	0.0	0.0	0.0
11.3	11.3	41.2	0.0	0.0	0.0
0.0	0.0	0.0	43.3	0.0	0.0
0.0	0.0	0.0	0.0	15.5	0.0
0.0	0.0	0.0	0.0	0.0	15.5

Point group

point_group_type: 6/mmm

Visualize Phonons here

Phonon mode (cm^{-1})	Representation
-0.0465217481	None
-0.0362848079	None
0.0136711726	A2u I
22.1183439196	E2g R
35.3915249465	B2g
112.721031921	E2u
114.212804132	E1g R
166.789595244	B1u
170.535305026	A1g R
226.002625615	E1u I
226.037033636	E2g R
275.946925877	A2u I
279.963912554	B2g



Read WARNINGS!

DFT Phonon mode 1x1x1 cell (cm^{-1})	DFT 1x1x1 Representation	Experimental modes	Experimental Representation	DFT Phonon modes for 2x2x2 cell	DFT 2 Represe
-0.13	Bu I			-0.58	Bu
-0.06	Au I			-0.04	Bu
-0.04	Bu I			0.06	Au
7.36	Bu I			6.08	Bu
25.80	Au I			24.65	Au
31.04	Bu I			26.09	Bu
76.66	Ag R			74.09	Ag
84.86	Ag R	80.56	Ag R	81.54	Ag
88.03	Bg R			87.63	Bg
90.32	Bg R			89.60	Bg
103.28	Bg R	96.54	Bg R	102.36	Bg
104.17	Bg R	108.32	Bg R	102.95	Bg
107.55	Au I			106.61	Au
108.54	Ag R			107.12	Ag
109.91	Au I			108.66	Au
112.03	Ag R	112.8	Ag R	111.10	Ag
114.06	Bu I			115.46	Bu
122.27	Bu I			121.19	Bu
124.29	Ag R			121.90	Ag
126.27	Ag R	129.2	Ag R	123.58	Ag
129.64	Bu I			126.25	Bu
134.19	Bu I			130.53	Bu
151.35	Ag R			150.19	Ag
156.27	Ag R	163.32	Ag R	153.05	Ag
175.28	Au I			176.42	Au
175.94	Au I			176.93	Au
184.24	Bg R			181.76	Bg
186.30	Bg R	191.64	Bg R	185.04	Bg
190.81	Bu I			189.22	Bu
190.93	Bu I			189.61	Bu
236.52	Ag R			234.90	Ag
239.60	Ag R	248.45	Ag R	239.42	Ag
252.88	Ag R	258.61	Ag R	250.04	Ag
253.04	Ag R	263.34	Ag R	252.26	Ag
264.26	Bu I			264.26	Bu
265.13	Bu I			264.73	Bu

- Experimental data from Ryan Beams, NIST
- <9% error, Beams et al., ACS Nano, 10 (10), 9626 (2016)

Email: kamal.choudhary@nist.gov

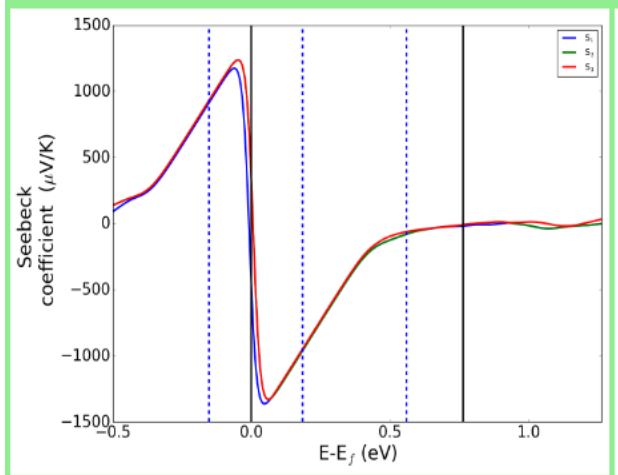
Thermoelectric properties

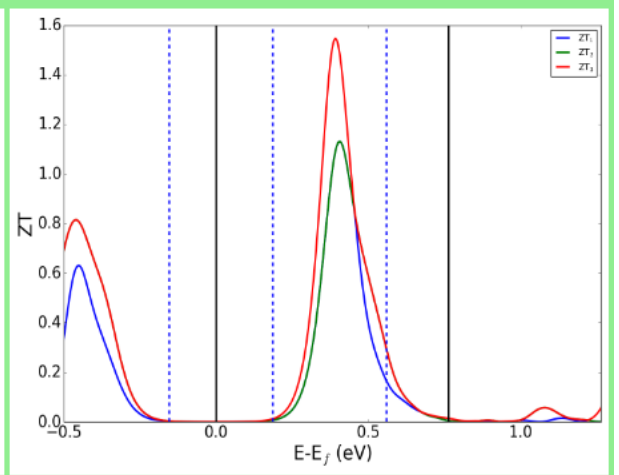
Electron mass tensor (m_e unit)

0.579472673637 -1.9247905275e-18 8.58074633074e-20
-1.9247905275e-18 0.579471339037 6.18803965953e-20
8.58074633074e-20 6.18803965953e-20 0.315280035074

Hole mass tensor (m_e unit)

1.18849079687 1.90402904433e-17 -6.32134631695e-19
1.90402904433e-17 1.18848809009 7.02149023383e-18
-6.32134631695e-19 7.02149023383e-18 1.90003598009





Temp-100 K | Temp-300 K | Temp-600 K

- BoltzTrap code in pymatgen
- Constant relaxation time approximation
- Only electronic contribution to thermal conductivity
- Perturbation in Fermi-distribution

$$f_0(\mathbf{r},\mathbf{k}) = \frac{1}{1+e^{\frac{E(\mathbf{k})-\mu}{k_B T}}} \qquad f = f_0 + f_1.$$

For a stationary near-equilibrium distribution, the Boltzmann equation is

$$\frac{df}{dt} = 0 = \frac{\partial f}{\partial t} + \nabla_{\mathbf{r}} f \cdot \frac{\partial \mathbf{r}}{\partial t} + \nabla_{\mathbf{k}} f \cdot \frac{\partial \mathbf{k}}{\partial t} + \left.\frac{\partial f}{\partial t}\right|_{scat.},$$

$$ZT = \frac{S^2\sigma}{\kappa} T, \quad \kappa = \kappa_e + \kappa_L$$

- Doping dependent properties for:
  Hall tensor, thermal conductivity,
  electronic conductivity tensor, Seebeck tensor

(UNDER CONSTRUCTION)

Email: kamal.choudhary@nist.gov

Read WARNINGS!

http://www.diss.fu-berlin.de/diss/servlets/MCRFileNodeServlet/FUDISS_derivate_000000017259/Lukas_Hammerschmidt.Thesis.pdf

Providing References to other databases

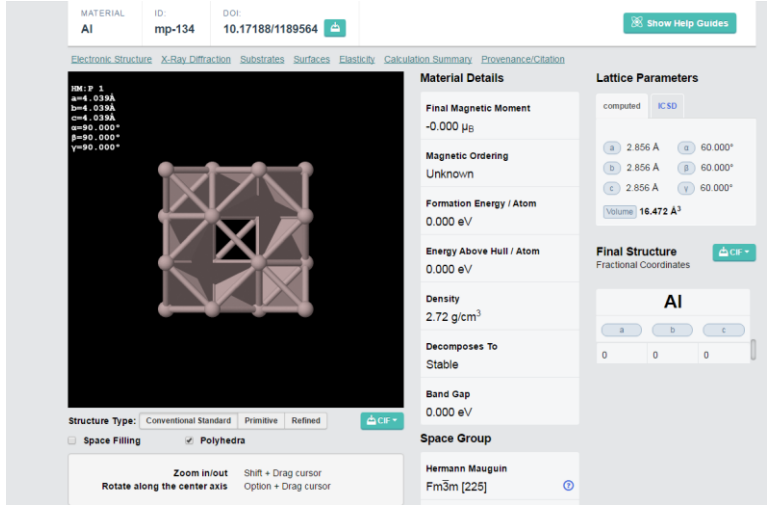
Reference

mp-134

ICSD-ID: 150692

AFLOW link

MP link



Email: kamal.choudhary@nist.gov

Summary Part-2

- New publicly available database specially dedicated to 2D materials (both bulk and single layer)
- Simple criteria to identify 2D materials, Nanowires and Quantum dots?
- 2D-2L, piezoelectric properties, defects and interface properties on the way
- Largest dataset for optical materials, easy screening of materials, characterizing nature of optical transitions
- Many-body effects (GW,BSE), Nonlinear optical properties on the way
- JARVIS-DFT data will be available in Citrine database soon
- We welcome your experimental data for validation !

Email: kamal.choudhary@nist.gov

JARVIS-ML

- 3A Introduction
- 3B Implementation using current methods
- 3C New hybrid ML + FF

Email: kamal.choudhary@nist.gov

3A Intro Machine Learning

- Learning == Dimensionality reduction
- No one knows the Potential Energy Surface (PES) : Need of ML

- Similarly, for materials == linear combination of features
- Very simple examples for feature selection:

  X: input data, say NaCl: [mean of atomic radii of constituents, electronegativity, atomic mass,….]

  Y: target data: [heat of formation, bulk modulus, bandgap,……]

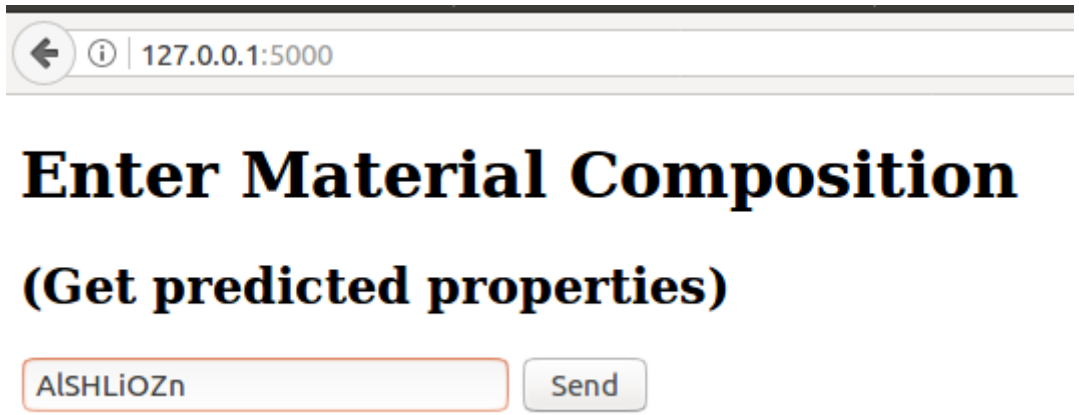
  Machine-Learning packages : Scikit-learn (Google), Tensor-flow (Google), Theano (Université de Montréal ,Canada)

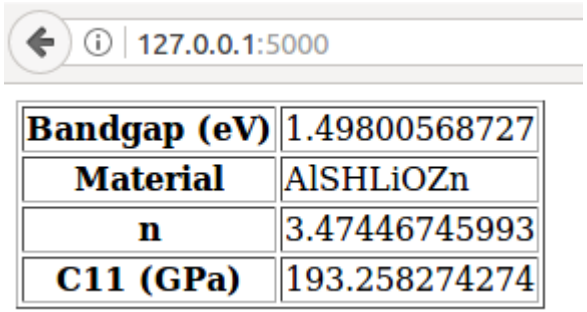
  Train a machine learning model with Neural network, linear regression, random-forest etc.

  For new material say (KCl), convet in the format of X, then query the model

Email: kamal.choudhary@nist.gov

3B Example using JARVIS-DFT data



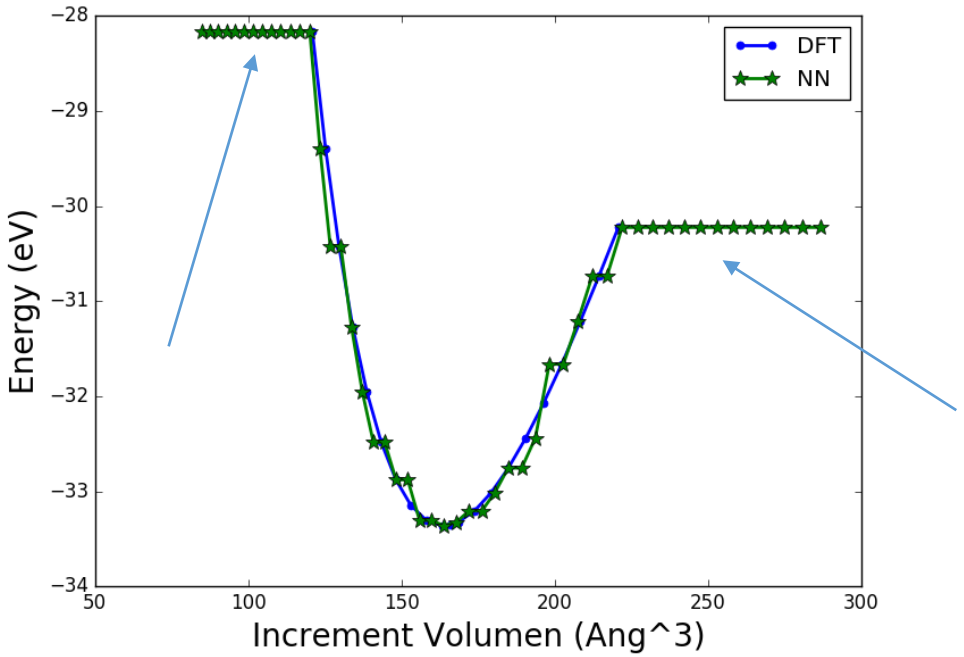


- Bandgap, refractive index elastic constant for example
- Currently running on my computer, testing and debugging may take several months

Email: kamal.choudhary@nist.gov

3C Artificial Neural network + FF

- Present trend: Thousands of DFT calculation, structure-property(energy) relationship, parametrize force-fields, limited to what we train—wrong extrapolation features! (E-V curve)
- Attempt to make new force-field: Machine-learning+FF-contribution (LJ, EAM, COMB and so on), Machine learning for interpolation, Physics for extrapolation
- ~500 DFT calculations for training database



For any atom i, we define the parameter

$$v_i^{(0)} = \frac{1}{\sigma^3} \sum_{j \neq i} e^{-r_{ij}^2/\sigma^2} f_c(r_{ij}),$$

where $f_c(r)$ is a truncation function defined by

$$f_c(r) = \begin{cases} \dfrac{(r - r_c)^4}{d^4 + (r - r_c)^4} & r \leq r_c \\ 0, & r \geq r_c. \end{cases}$$

*Notes Yuri Mishin

Email: kamal.choudhary@nist.gov

DEMO !

Email: kamal.choudhary@nist.gov

Conclusions and Future work

- New publicly available databases!
- Simply Google "JARVIS-DFT", "JARVIS-FF" or browse http://www.ctcms.nist.gov/~knc6/JARVIS.html
- Identification and characterization of new/existing materials using classical and quantum methods
- Flexible python framework to accommodate other models as well: CALPHAD, FEM, PF; golden time for Multi-scale modelling
- Need of your **Experimental data** for validation!
- Soon JARVIS will be available on smart-phones with voice-recognition apps!
- JARVIS-Wiki for documentation, and Hands-on tutorials will be available soon

JARVIS for YOU !

THANKS FOR YOUR ATTENTION !

Email: kamal.choudhary@nist.gov