NIST
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U.S. Department of Commerce

JARVIS-ML

2D/3D materials screening and genetic algorithm with ML model

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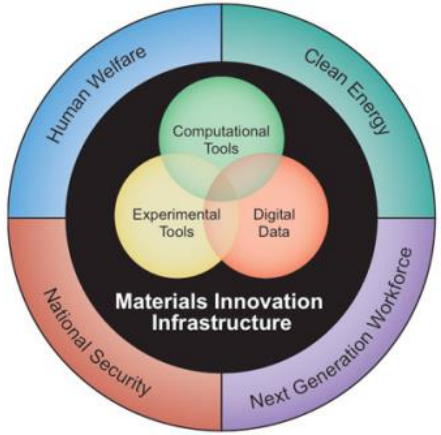
University of Maryland

August 02, 2018



JARVIS

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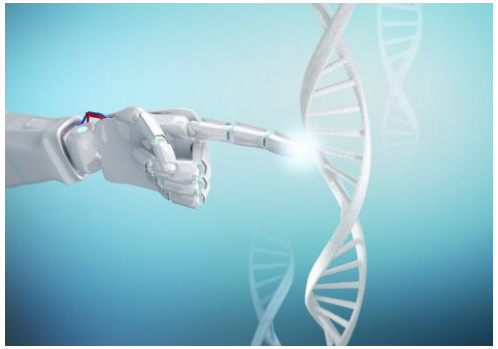
Outline

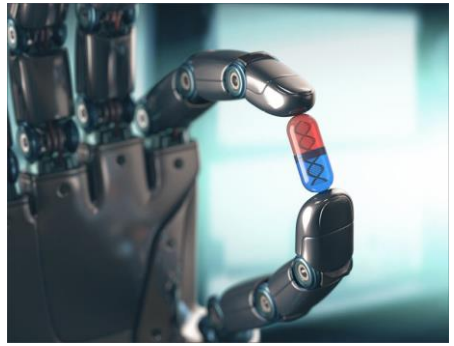
- AI in materials, Motivation
- JARVIS-FF, DFT and ML
- Representing materials to computers
- Visualizing multi-dimensional data
- Histograms for target data
- Gradient boosting decision trees
- Classification and regression models, feature importance
- Application of ML models in materials screening
- Application of ML in mapping energy landscape
- Web-app
- Conclusions

AI in materials

- For successful application of AI:

  -High fidelity data, pertinent algorithm and validation strategy
- Unlike other AI input data (cat/dog images from facebook etc.), materials data are really small and takes long time to generate
- Available of easily applied AI algorithms: scikit-learn, tensor-flow, lightgbm, Keras etc.
- Publicly available databases such as JARVIS-DFT, Materials-project, AFLOW, OQMD, Harvard clean energy project, AiiDA, PDB database, COD database etc.
- Immense potential for AI in materials: medicine-design, medical-diagnosis, alloy-design,…

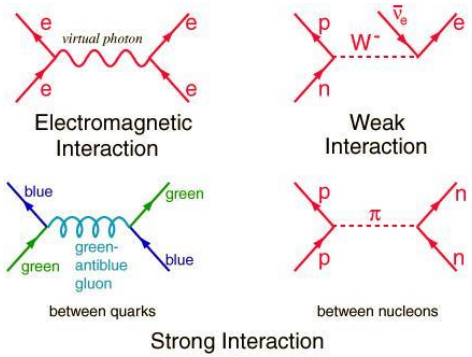


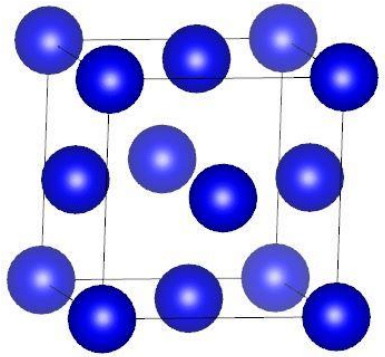


https://www.youtube.com/watch?v=8r_smb-9GTg
https://www.nesgt.com/blog/2016/10/how-artificial-intelligence-is-being-used-in-the-pharmaceutical-industry
https://rowanalytics.com/blog-post/ai-in-medicine-a-historical-perspective/

Motivation

- Bridge gap between AI and materials community
- 10^{100} materials predicted, impossible to characterize with current theoretical and experimental techniques
- Fully automated computational and experimental discovery as well as industrial implementation
- Learning data from classical-physics and quantum-physics based outputs through AI/machine learning techniques
- JARVIS : **J**oint **A**utomated **R**epository for **V**arious **I**ntegrated **S**imulations

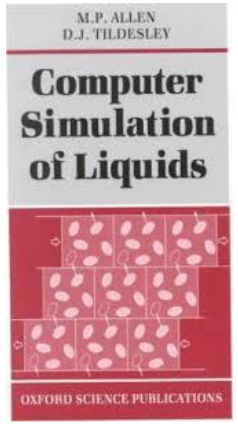




https://en.wikipedia.org/wiki/Iron_Man
https://nige.wordpress.com/2008/01/30/book/interactions/
https://arxiv.org/abs/1805.07325

JARVIS-FF

Force-field (classical)



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

- **Solve Newton's equation for atomic positions**
- **Approximations for V (force-fields)**:

EAM, EIM, MEAM, AIREBO, REAXFF, COMB, COMB3, TERSOFF, SW *etc.*

- **Contains:**

Automated LAMMPS based force-field calculations on DFT geometries. Some of the properties included in JARVIS-FF are energetics, elastic constants, surface energies, defect formations energies and phonon frequencies of materials

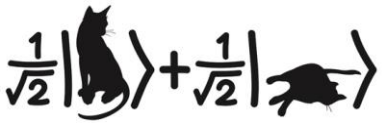
- **Time:** Takes years to fit FFs, relatively quick calculations
- **Website**: https://www.ctcms.nist.gov/~knc6/periodic.html
- **Publications**:

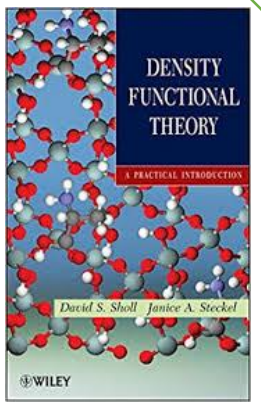
➢ Nature:Scientific Data 4, 160125 (2017)
➢ arXiv:1804.01024 (2018)

JARVIS-DFT

Density-functional theory (quantum)

Schrödinger's cat





$$H\psi = E\psi$$

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

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

- **Solve Scrodinger equation for electrons**
- >30,000 materials data (3D, 2D, 1D, 0D)
- **Contains:**

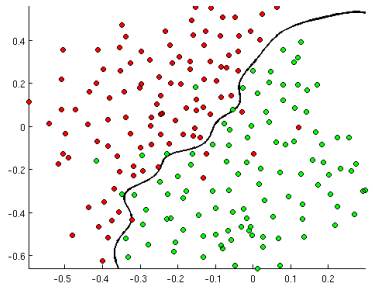
Formation energy, exfoliation energy, diffraction pattern, radial distribution function, band-structure (SOC/Non-SOC), density of states, carrier effective mass, temperature and carrier concentration dependent thermoelectric properties, elastic constants and gamma-point phonons

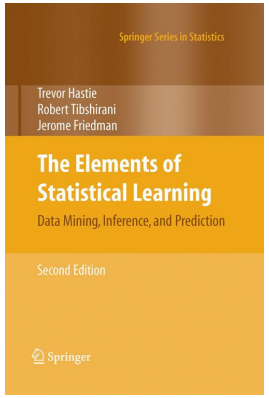
- **Time:** 5000 cores for last 4 years
- **Website**: https://www.ctcms.nist.gov/~knc6/JVASP.html
- **Publications**:

➢ Nature:Scientific Reports 7, 5179 (2017)
➢ Nature:Scientific Data 5, 180082 (2018)
➢ Phys. Rev. B 98, 014107 (2018)

JARVIS-ML

Machine learning (data-driven)





- **Drawing the line, dimensionality reduction, curve-fitting?**
- Neural nets, decision trees, fuzzy-logic etc.
- Uses gradient boosting decision tree
- **Contains:**

Machine learning prediction tools, trained on JARVIS-DFT data.

Some of the ML-predictions focus on energetics, heat of formation, GGA/METAGGA bandgaps, bulk and shear modulus, exfoliation energy, refractive index, magnetic moment, carrier effective masses

- **Time:** Much easier and faster to train
- **Website**: https://www.ctcms.nist.gov/jarvisml/
- **Publication**:

➢ Accepted Phys. Rev. Mat. (2018)

JARVIS

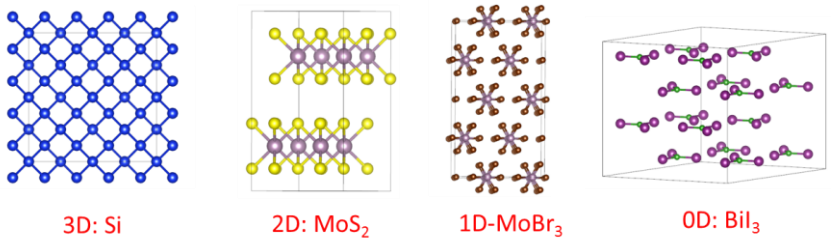
JARVIS-DFT data

- Large and reliable dataset of
  - ➢ optoelectronic properties (>18000)
  - ➢ Elastic properties (>11000)
  - ➢ 2D/1D/0D exfoliation energies (>800)
  - ➢ Topological material properties, Z_2 index (>2000)

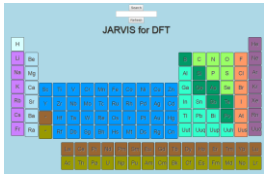
and others…

Dimensionality of materials

- **>700 2D mono/multi-layers & >30000 3D bulk materials**
- **Increasing ~3000 materials/month**

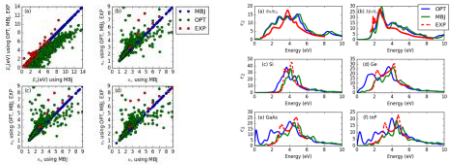


Webpage: https://jarvis.nist.gov



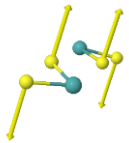
Optoelectronic properties

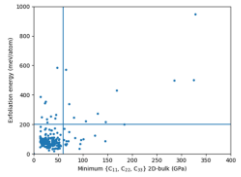
- **OptB88vdW, TBmBJ and HSE06 bandgaps**
- **Frequency dependent dielectric functions**

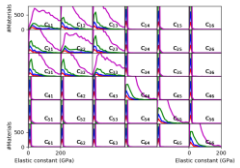


Elastic properties

- **6x6 elastic tensors, Poisson's ratio and phonons**

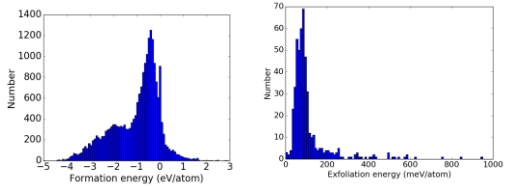






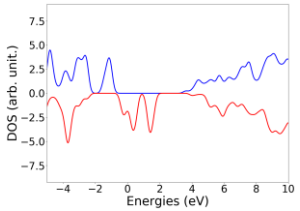
Energetics

- **Enthalpy of formation and enthalpy of exfoliation**
- **Exfoliable materials: <200 meV/atom**



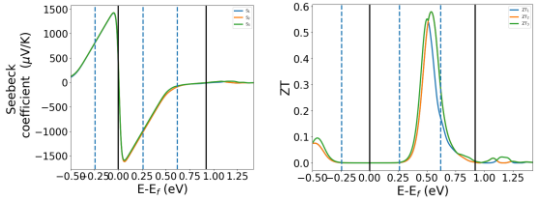
Magnetic properties

- **Magnetic moments**

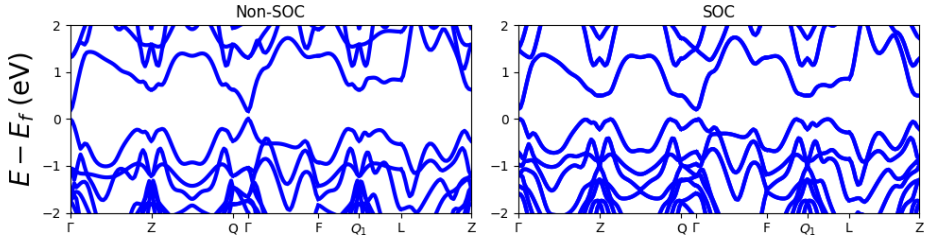


Transport properties

- **Carrier effective mass, Seebeck coefficient and zT**



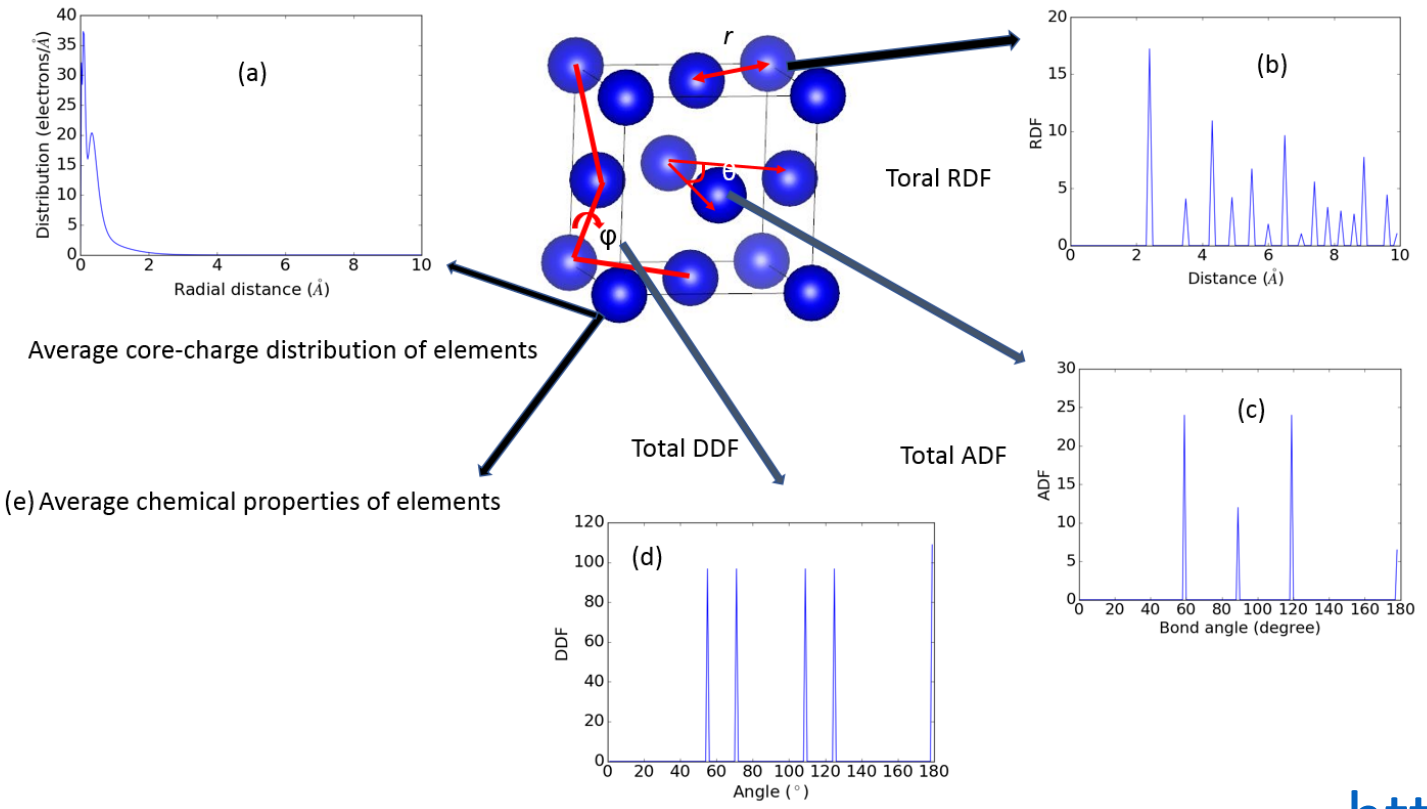
Topological properties



Steps in JARVIS-ML model

1) Descriptor selection (perhaps the most important step!),visualization
2) Preprocessing (variance threshold, PCA etc.)
3) Train-test split of data (90%-10% for instance)
4) Hyperparameter optimization using grid-search on train data
5) Select the best model (based on R^2/**MAE**/RMSE accuracy)
6) Prediction on test data (classification/regression)
7) Plot learning curve for complexity analysis
8) Plot feature importance (if available)

Finding the right features/descriptors: representing atomic structure to computers

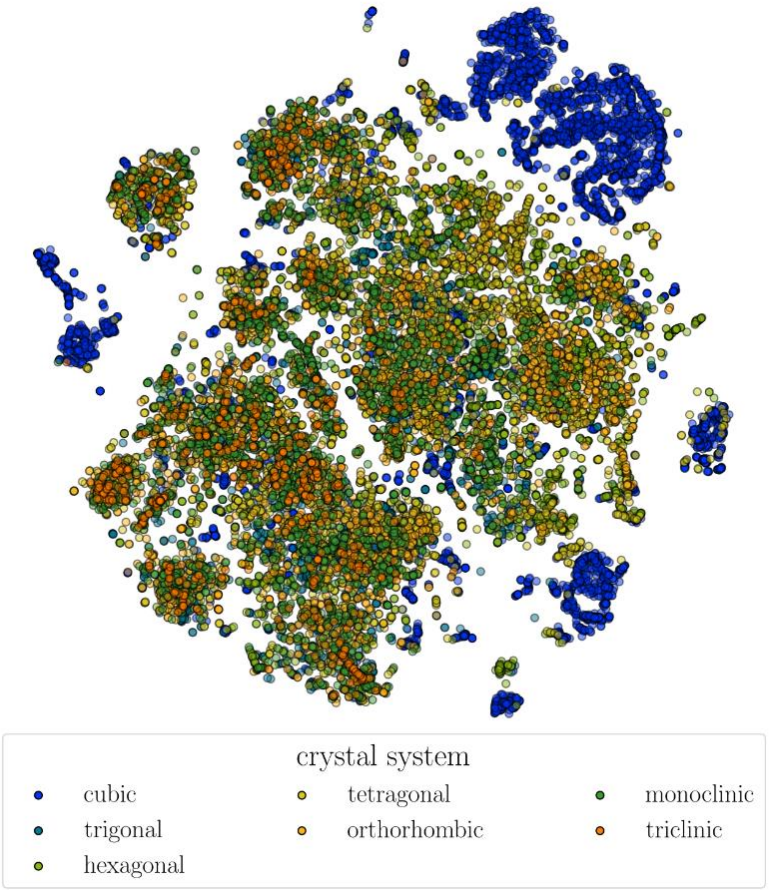


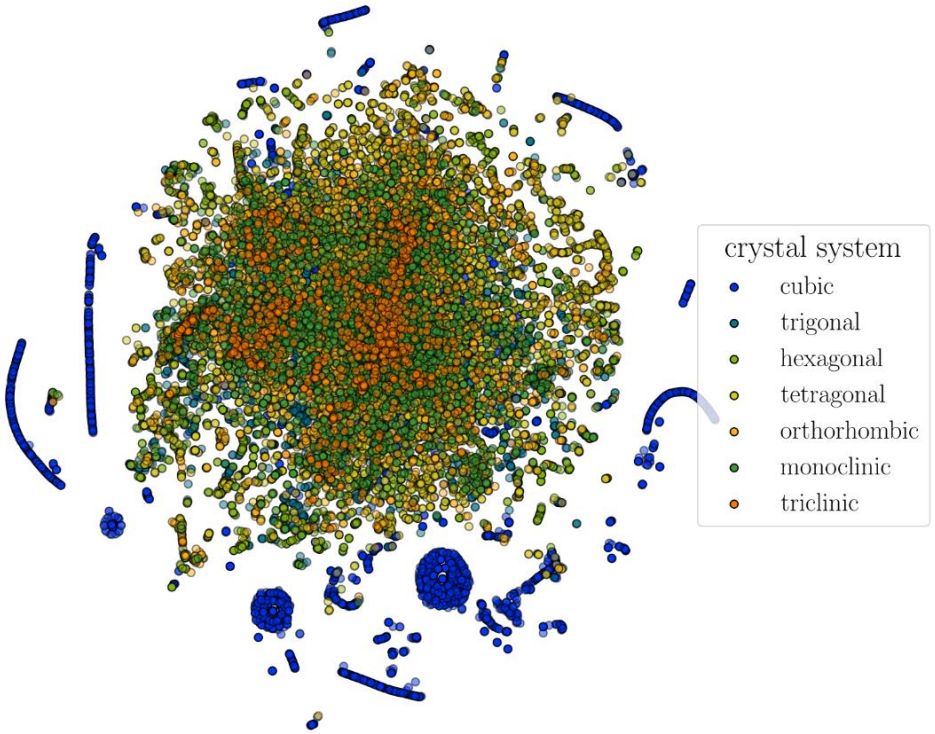
- Arithmetic operations (mean, sum, std. deviation…) of **electronegativity, atomic radii, heat of fusion**,….
of atoms at each site
(example: Electronegativity of Mo+Mo+S+S+S+S)/6 = 0.15
- Atomic bond distance based descriptors
- Angle based descriptors

1557 descriptors/features for one material

https://github.com/usnistgov/jarvis

Visualizing multi-dimensional data with t-SNE



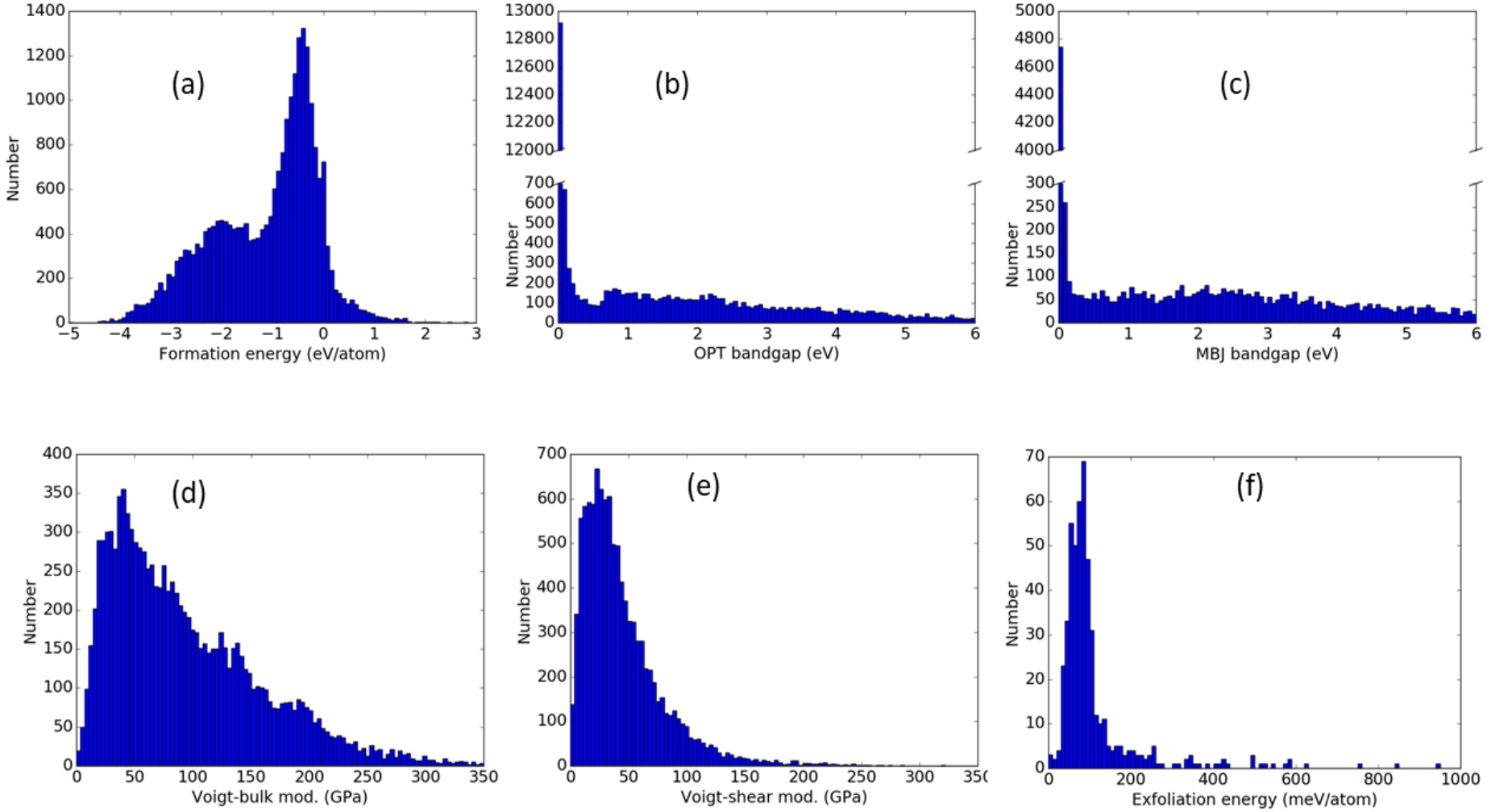


- Converts similarities between data points to joint probabilities
- Visulaization with t-SNE for ~25000 materials

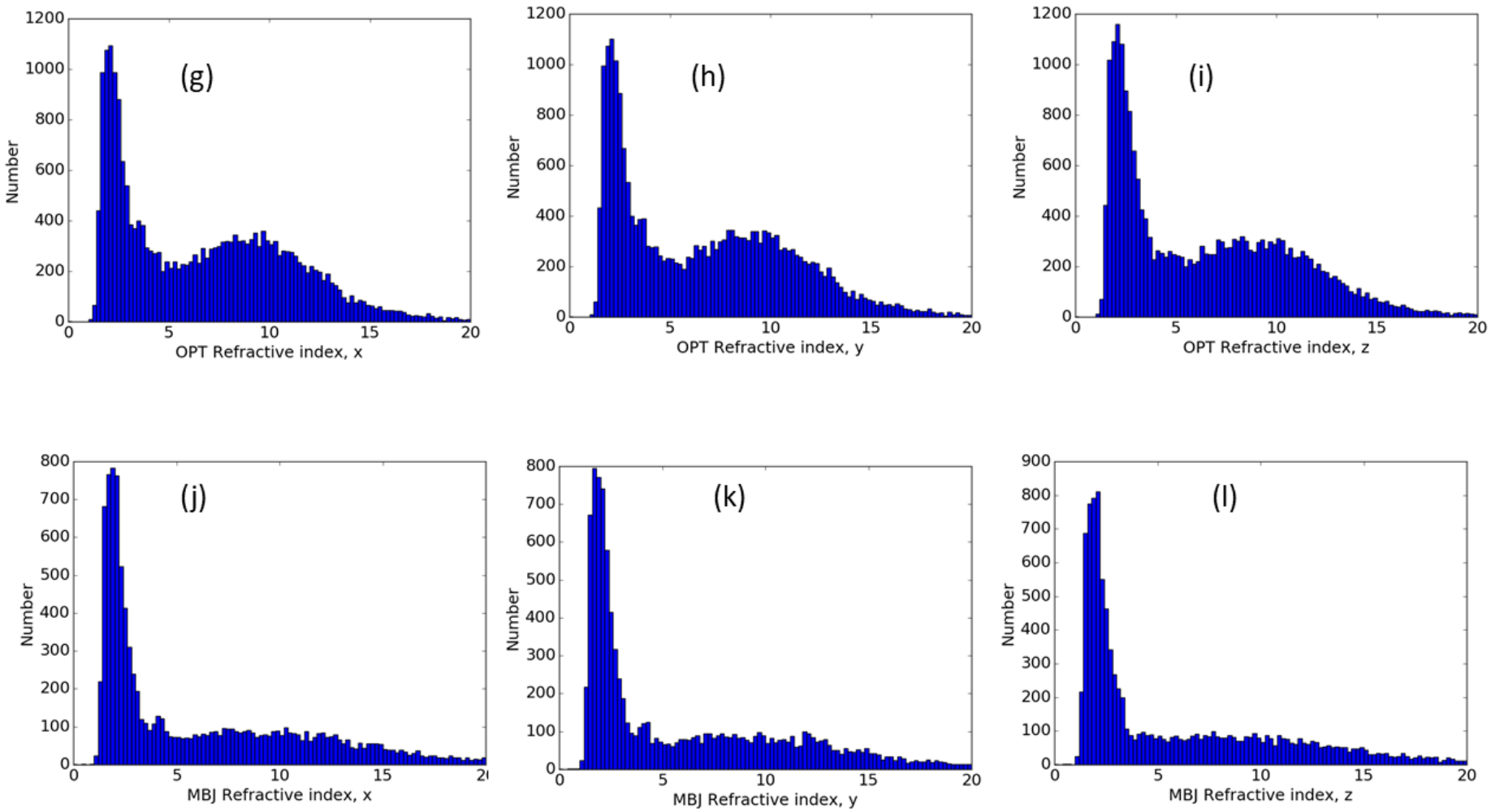
http://holoviews.org/
http://scikit-learn.org/stable/modules/generated/sklearn.manifold.TSNE.html

Data-spread: histograms

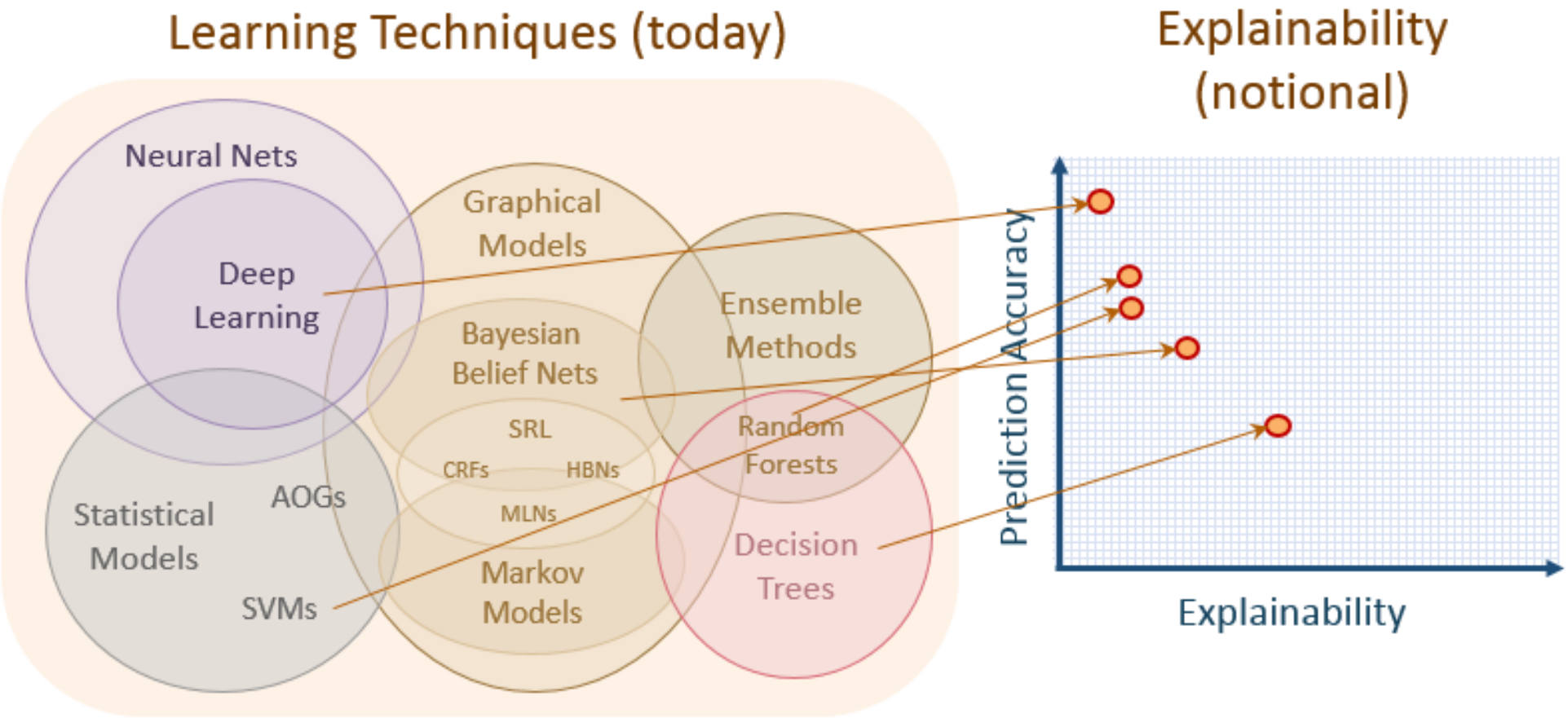
- Identifying the range of target data
- Energetics, electronic, optical, and mechanical properties
- AI generally good for interpolation



Data-spread: histograms



Need of explainable AI for materials: black box may not work for materials community



https://www.darpa.mil/program/explainable-artificial-intelligence

Gradient boosting decision tree (GBDT)

- Ensemble of weak decision tree models
- Consecutively fits new models to provide a more accurate estimate of the response variables
- Suppose there are *N* training examples: $\{(x_i, y_i)\}^N$
- GBDT model estimates the function of future variable *x* by the linear combination of the individual decision trees using:

$$f_m(x) = \sum_{m=1}^{M} T(x; \theta_m)$$

where $T(x; \theta_m)$ is the *i*-th decision tree, θ_m is its parameters and *M* is the number of decision trees

- Final estimation in a forward stage-wise fashion

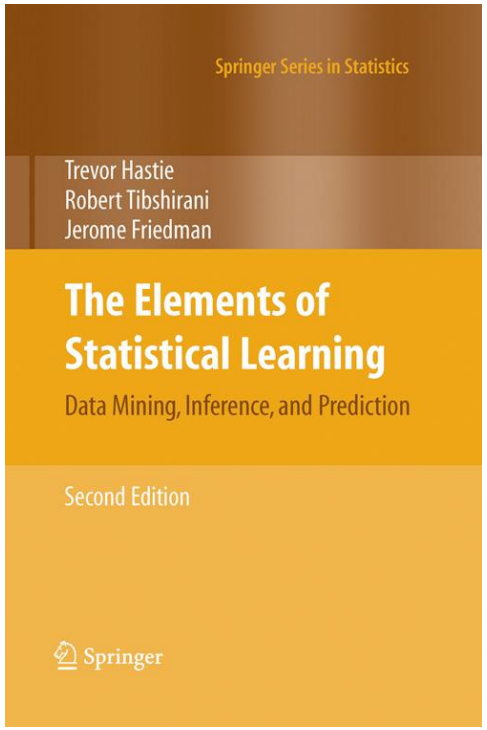
$$f_m(x) = f_{m-1}(x) + T(x; \theta_m)$$

where $f_{m-1}(x)$ is the model in $(m-1)$ step. The parameter θ_m is learned by the principle of

- Empirical risk minimization using:

$$\widehat{\theta_m} = arg\,\underset{\theta_m}{min} \sum_{i=1}^{N} L\big(y_i, f_{m-1}(x) + T(x; \theta_m)\big)$$

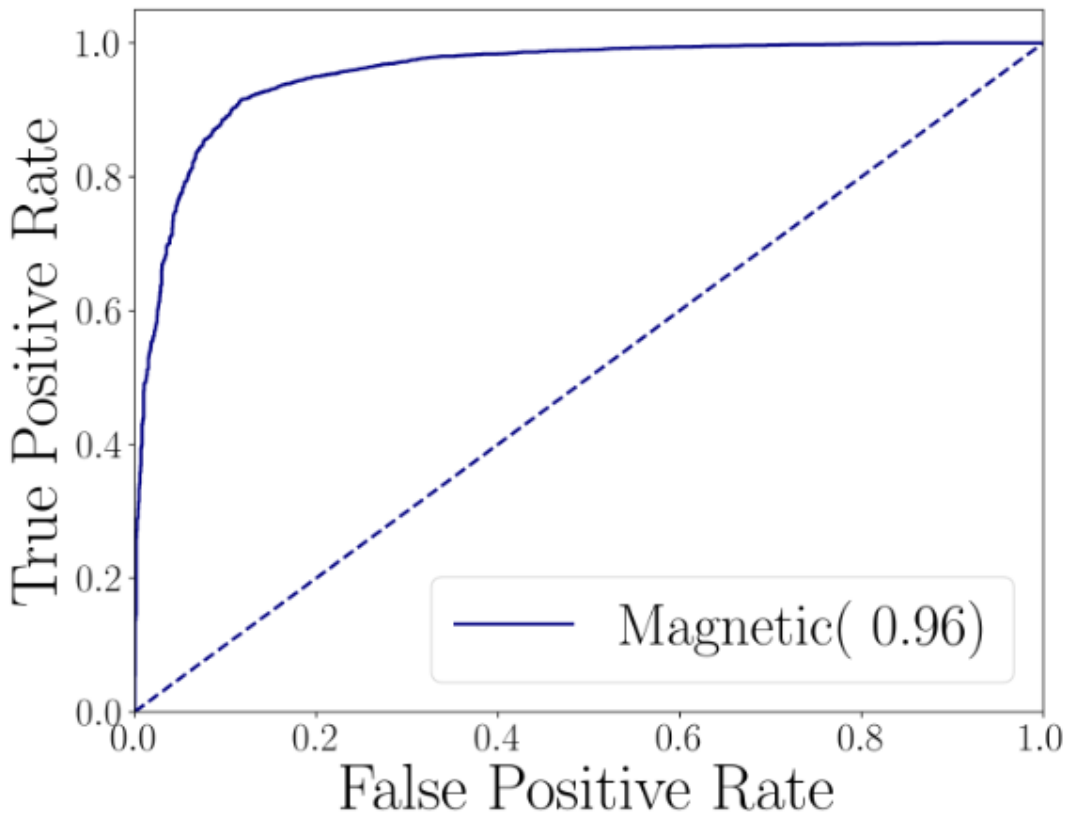
where *L* is the loss-function.

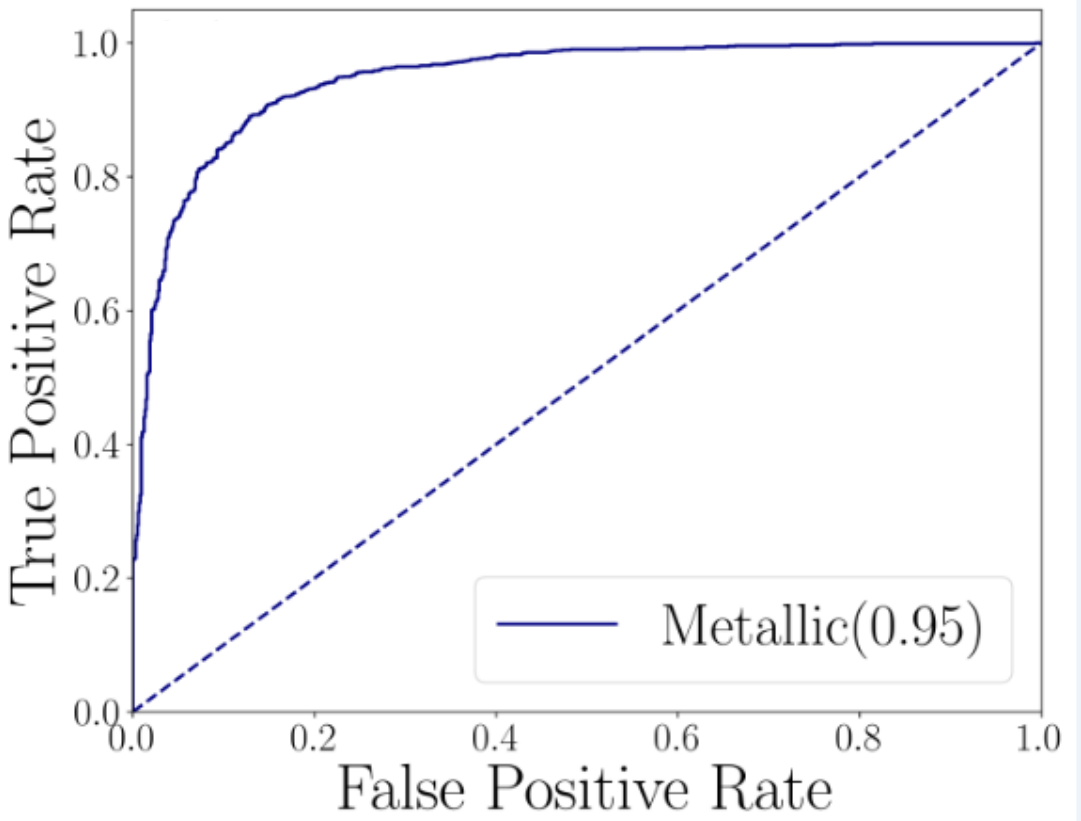


https://web.stanford.edu/~hastie/Papers/ESLII.pdf

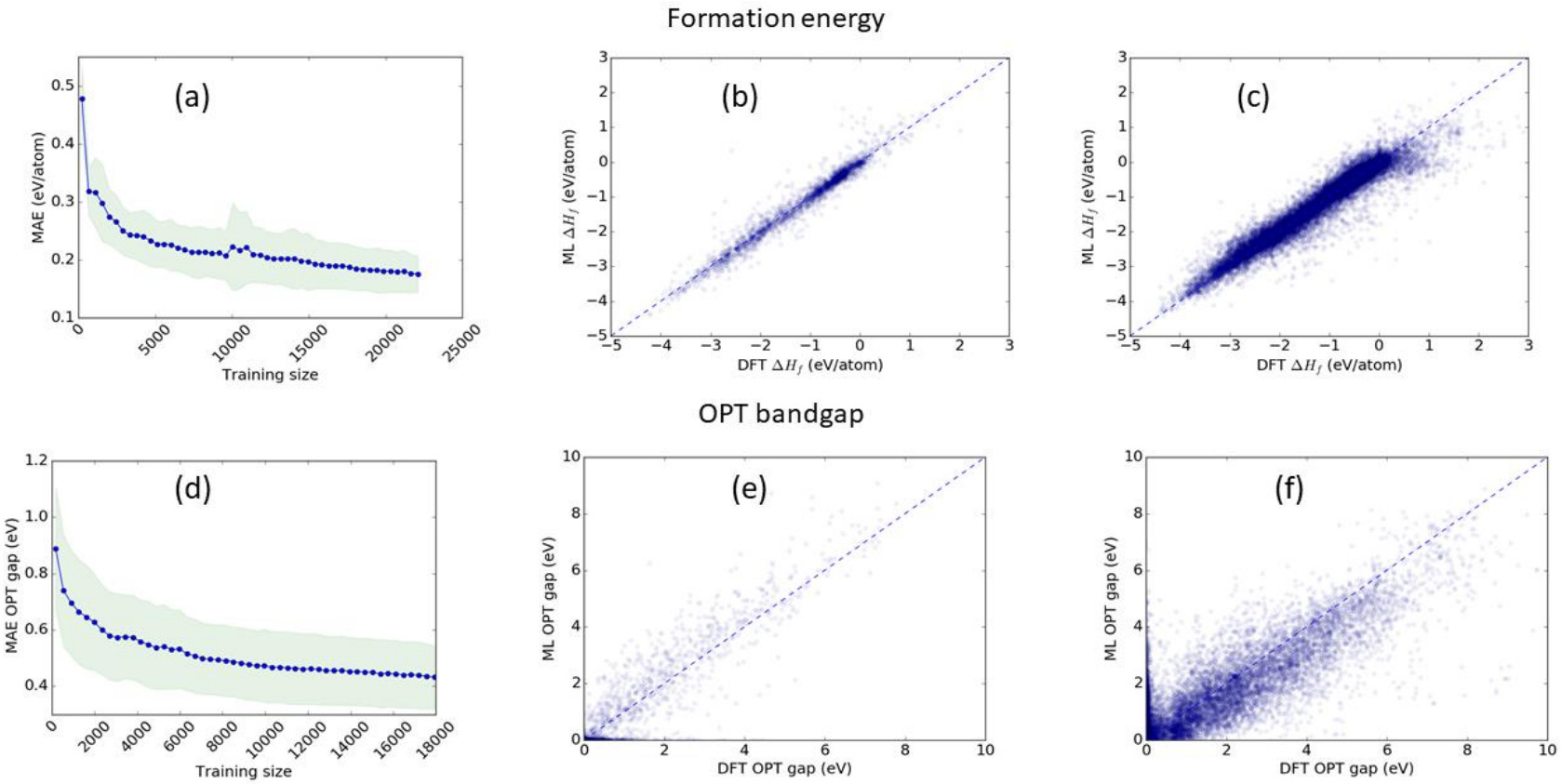
Classification problem: metal/non-metal, magnetic/non-magnetic materials

ROC-curve: Excellent classification models





Regression models: formation energy and bandgap model



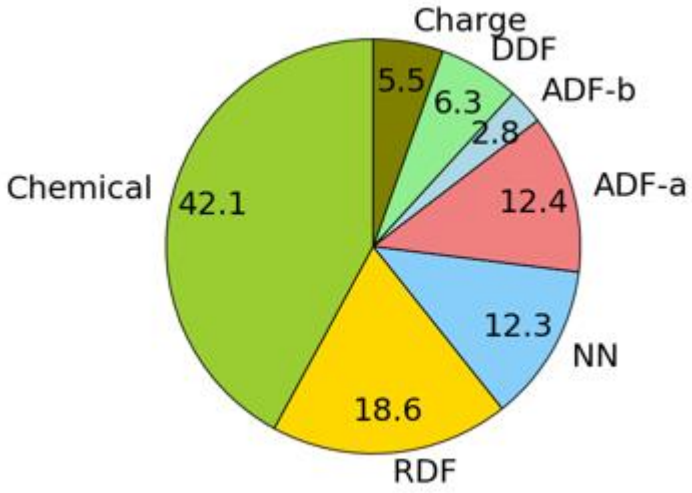
Learning curve shows scope of further improvement

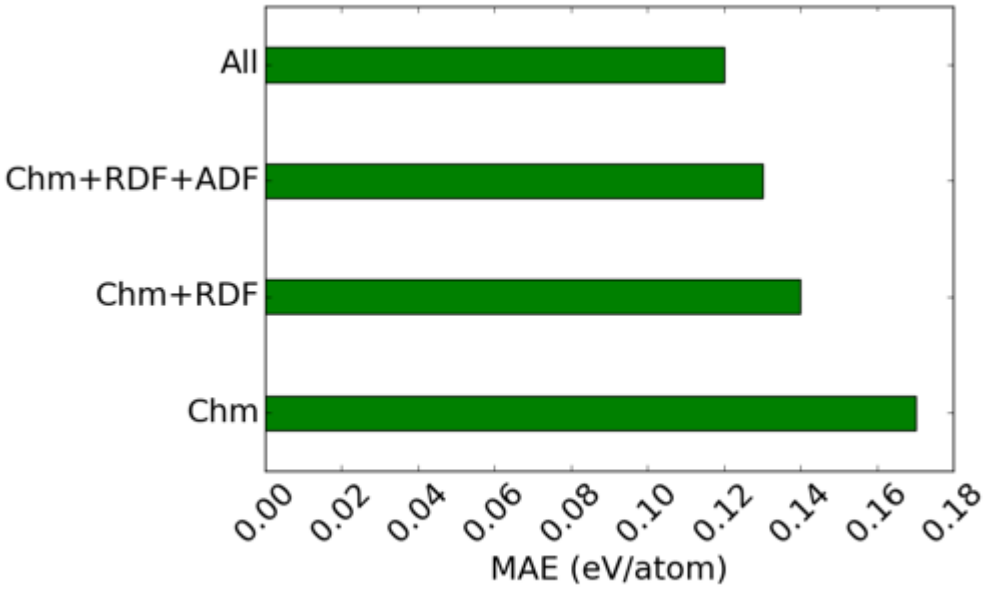
Other model performance

Property	#Data-points	$MAE_{CFID-DFT}$	$MAE_{DFT-Exp}$
Formation energy (eV/atom)	24549	0.12	0.136
Exfoliation energy (meV/atom)	616	37.3	-
OPT-bandgap (eV)	22404	0.32	1.33
MBJ-bandgap (eV)	10499	0.44	0.51
Bulk modulus (GPa)	10954	10.5	10.0
Shear modulus (GPa)	10954	9.5	10.0
OPT-n_x (no unit)	12299	0.54	1.78
OPT-n_y (no unit)	12299	0.55	-
OPT-n_z (no unit)	12299	0.55	-
MBJ-n_x (no unit)	6628	0.45	1.6
MBJ-n_y (no unit)	6628	0.50	-
MBJ-n_z (no unit)	6628	0.46	-

Performance on 10 % held data

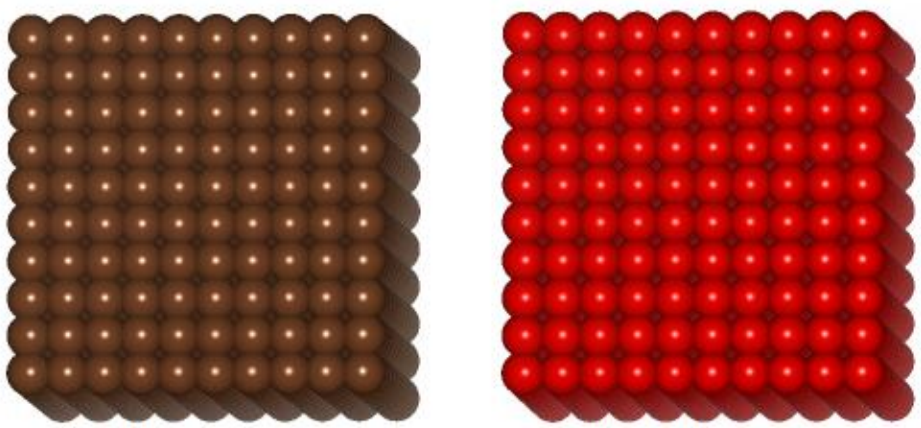
Explainability: feature importance





- Chemical features most important followed by RDF and NN
- Incrementally adding structural features decreases MAE

Introduction to Genetic Algorithm



(a) Artificial cubic parent structure. (b) Artificial cubic parent structure.

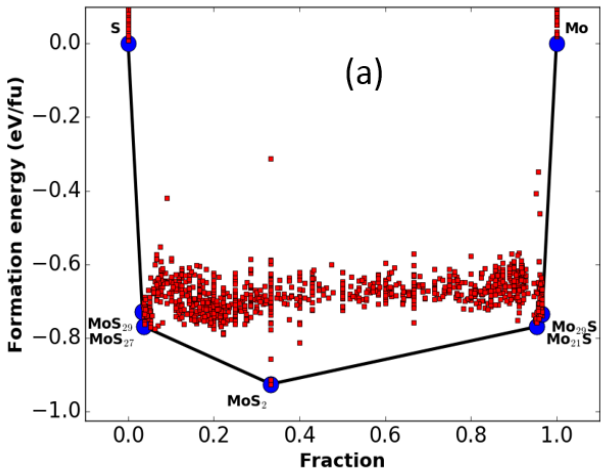
(c) Child created by the slicing crossover using a horizontal cut. (d) Child created by the slicing crossover using a periodic cut.

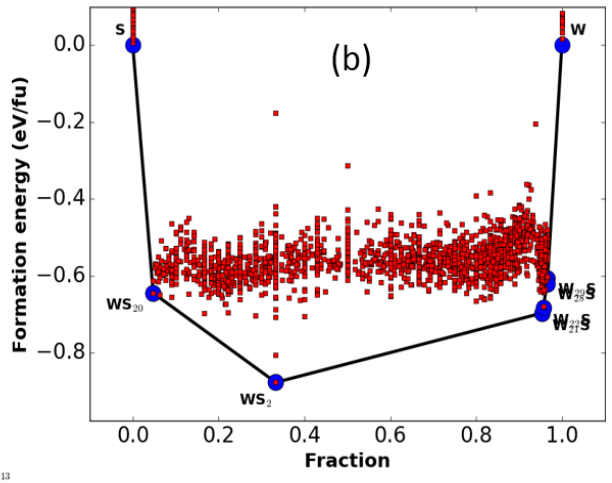
Picture from GASP manual

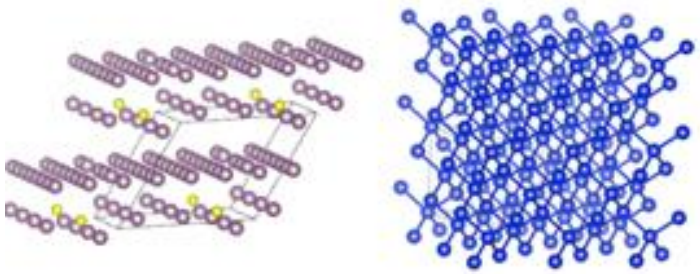
- Based on **'Survival of the fittest'** theory: fitness of crystal structure based on energy of structure
- Parents to offspring crystal structure
- Generally energy is obtained from DFT, MD…let's try ML ?

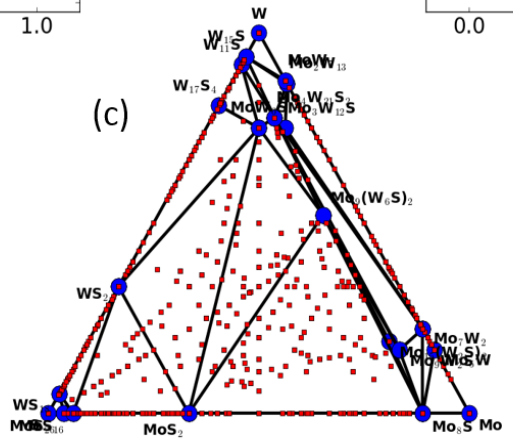
D. M. Deaven, Molecular geometry optimization with a genetic algorithm, Physical Review Letters, 75 (1995)
G. Ceder, Data-mining-driven quantum mechanics for the prediction of structure, MRS Bulletin, 31 (2006)
https://github.com/henniggroup/GASP-python/

Search for new materials: Genetic algorithm with ML





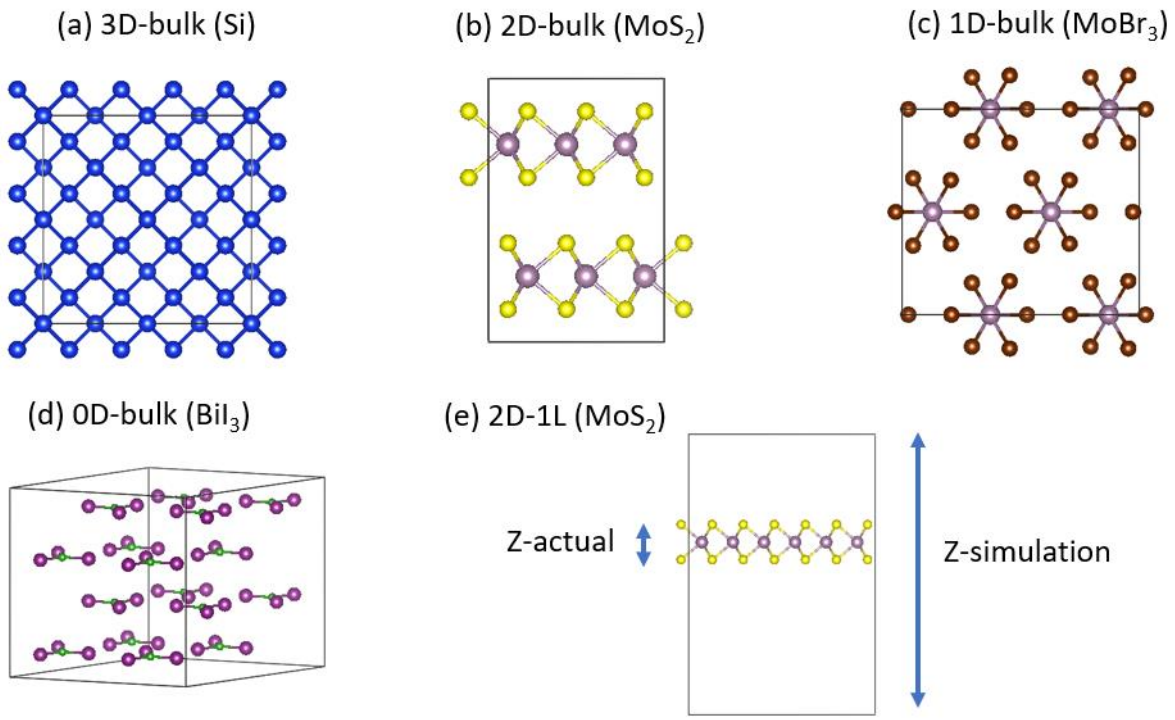




- New way of validating ML model for materials

- MoS_2, WS_2 indeed stable as in DFT and experiments
- Need further verification foor low-lying energy structures with DFT

2D materials screening: flexible electronics applications

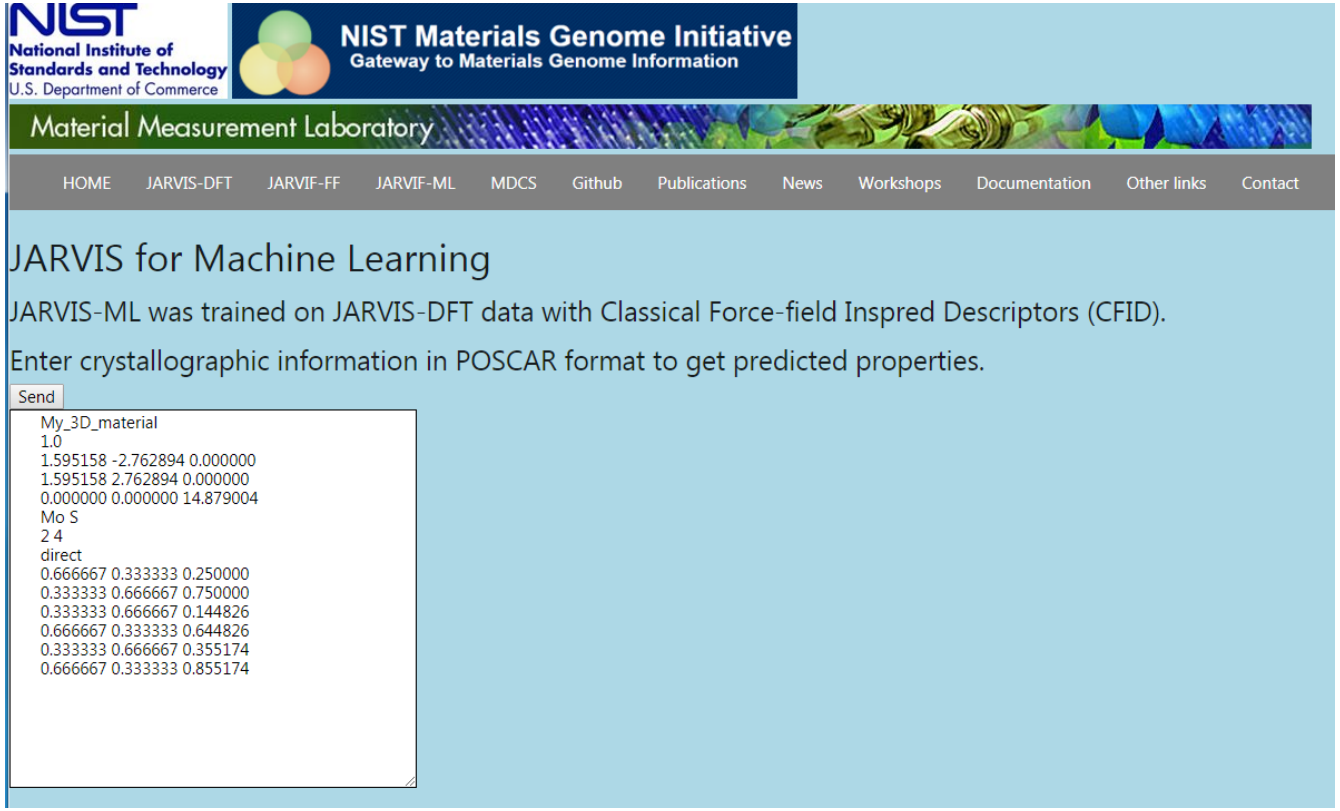


- ~5000 2D materials predicted
- Requires expensive DFT calculations for predicting properties such as bandgap, exfoliation energy etc.
- Use of ML drops down the time to a few seconds
- Using this technique we identified new 2D materials such as CuI, InS etc.
- Validated using DFT

Web-app: DEMO

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

- Pickle the learnt parameters
- Integrate with FlaskPython



Getting hands on: github sample trainng

https://github.com/usnistgov/jarvis/blob/master/jarvis/db/static/jarvis_ml-train.ipynb

https://github.com/usnistgov/jarvis/blob/master/jarvis/sklearn/examples/desc_example.py

usnistgov / jarvis

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Branch: master | jarvis / jarvis / db / static / jarvis_ml-train.ipynb | Find file | Copy path

JARVIS-Unifies jarvis-ml nb 75836d0 24 seconds ago

1 contributor

1054 lines (1053 sloc) 110 KB | Raw | Blame | History

Training a JARVIS-ML model

In [64]:

```
#from jarvis.sklearn.get_desc import get_comp_descp
from monty.serialization import loadfn, MontyDecoder,dumpfn
import numpy as np
from sklearn.metrics import mean_absolute_error,r2_score,mean_squared_error
import lightgbm as lgb
import matplotlib.pyplot as plt
plt.switch_backend('agg')
%matplotlib inline
import pandas as pd
from sklearn.datasets import load_boston
from sklearn.model_selection import train_test_split,learning_curve,cross_val_score,cross_val_predict,Grid
SearchCV,RandomizedSearchCV
import scipy as sp
import time,os,json,pprint
from sklearn.feature_selection import SelectKBest,f_classif,SelectFromModel,VarianceThreshold
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler


# Download descriptors and material data from the following link:
#  https://figshare.com/articles/JARVIS-ML-CFID-descriptors_and_material_properties/6870101

# Websites: https://www.ctcms.nist.gov/jarvisml, https://jarvis.nist.gov
# https://arxiv.org/abs/1805.07325


# NIST-disclaimer: https://www.nist.gov/disclaimer
```

On-going work

- Combining all materials data >5 million:
  solid-state crystals, molecules, proteins in one database and their visualization
- Multi-output Regression
- Active learning: train on DFT data, add to experiments to reduce domain search
- Transfer learning: Use previously trained model to learn on new data

Conclusions

- Golden time to integrate physics and data-science
- ML/AI as an aid to conventional theoretical methods such as DFT
- JARVIS bridging the gap between data-science and physics based models
- Providing unique material-descriptors
- All the code and data publicly available
- Formation energy convex hull plot as an example, other multicomponent systems also possible
- Web-app for on-the fly prediction of properties
- Immense potentials for electronics and biomedical industry
- Important links:

✓ https://jarvis.nist.gov/

✓ https://www.ctcms.nist.gov/jarvisml/

- E-mail: kamal.choudhary@nist.gov