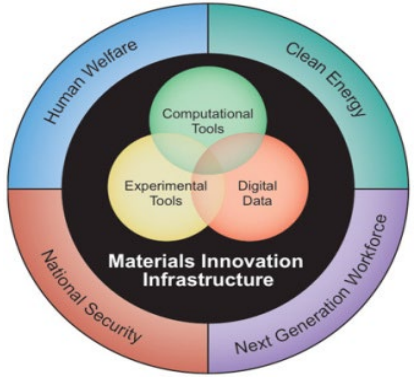
National Institute of Standards and Technology
U.S. Department of Commerce




# GNN for Materials Design

## Atomistic structure, Spectral, Image and Text data

Kamal Choudhary
https://jarvis.nist.gov/
NIST, Gaithersburg, MD, USA
APS 2023

JARVIS

**Joint Automated Repository for Various Integrated Simulations**

# Outline

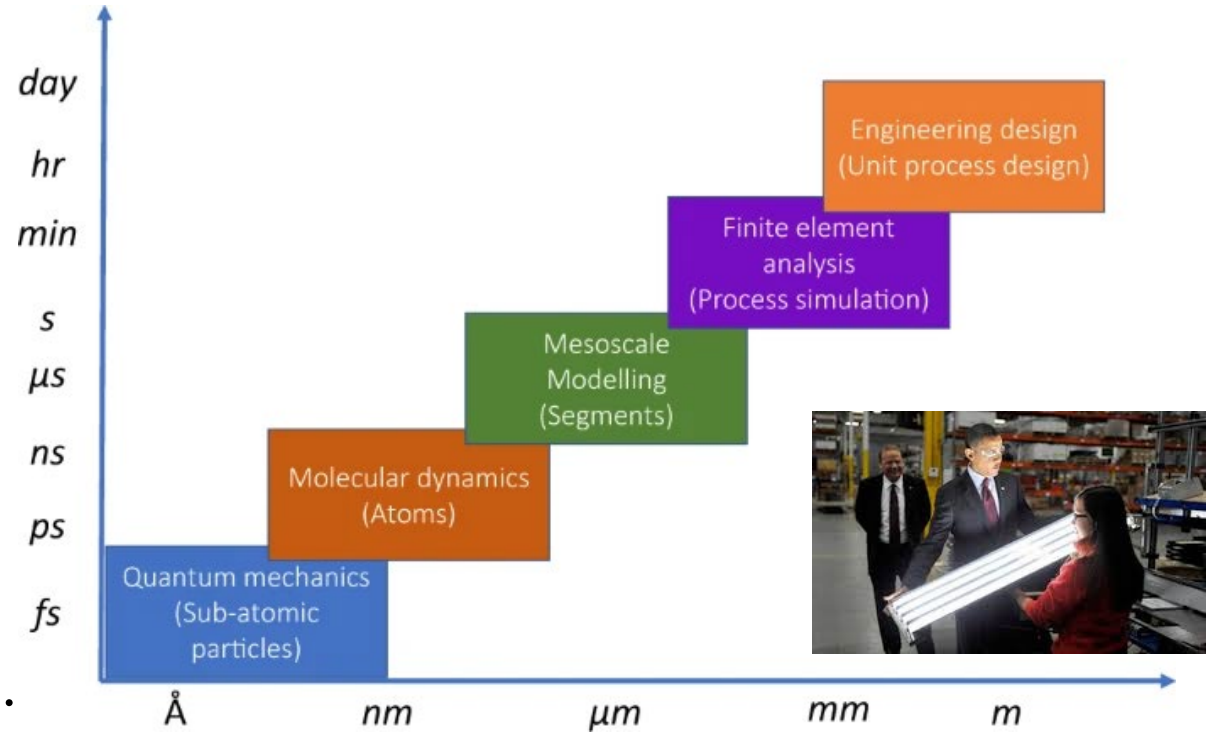
## Contents

- Motivation
- Introduction
- Electronic structure databases
- ALIGNN
- AtomVision
- ChemNLP
- Leaderboard
- Summary

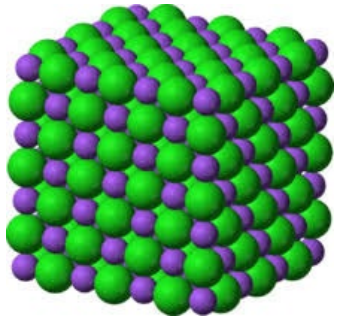
# Motivation

- Accelerate traditional computational and experimental methods
- Automate experimental data analysis,
- Discover new materials,
- Develop new methods,
- Find new physical equations/phenomenon,
- Enhance collaboration,
- Uncertainty quantification, reproducibility,.

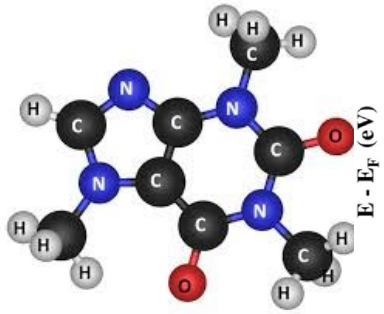
Modularity: discrete, continuous, images, text



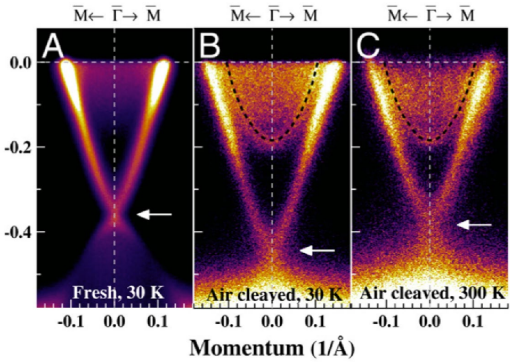

**Materials Genome Initiative 2011**



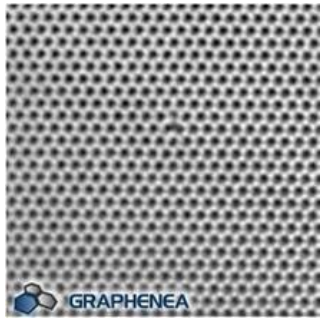
Crystals



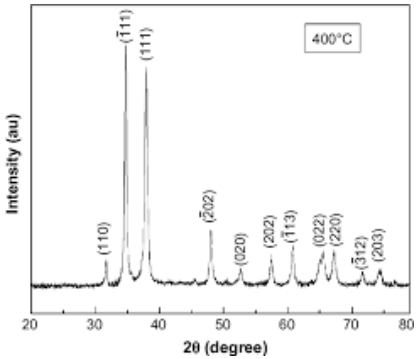
Molecules




Band-structure

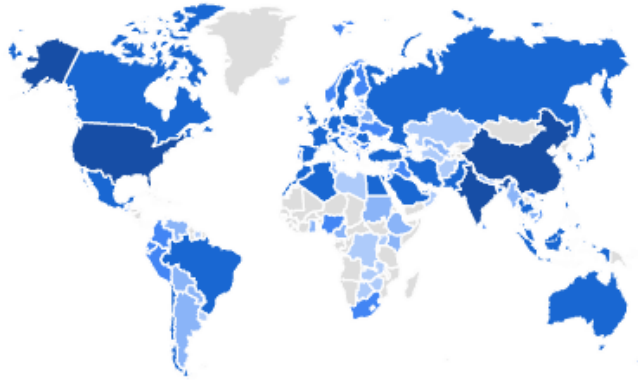



TEM images



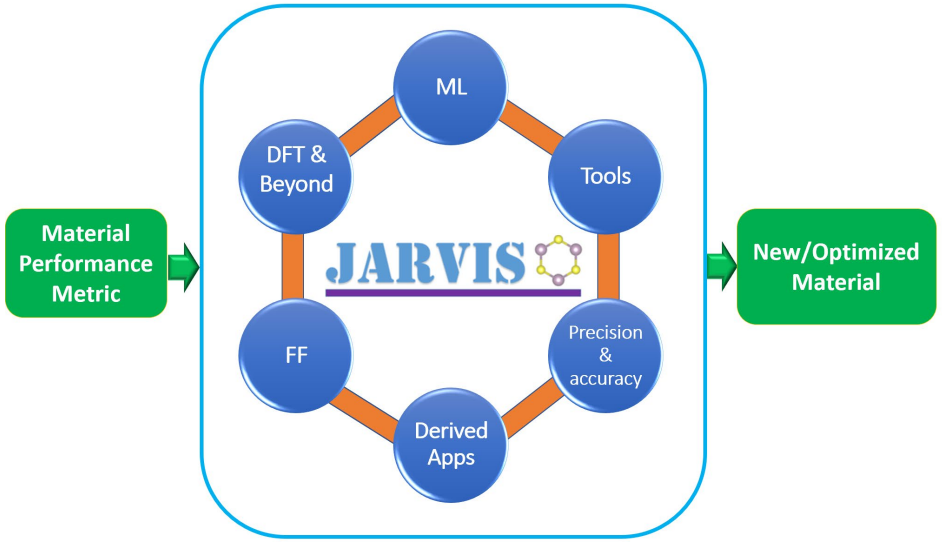

XRD spectra

# Databases, Tools, Events, Outreach



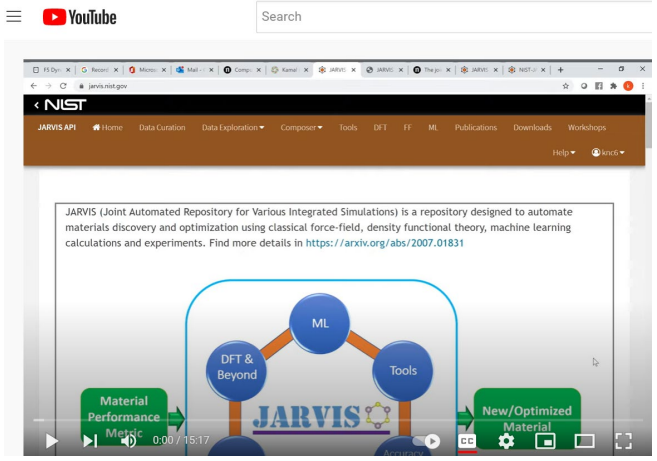
**https://jarvis.nist.gov**

Requires login credentials, free registration




**Established**: January 2017
**Published**: >40 articles
**Users**: >15000+ users worldwide
**Materials**: >70000, millions of properties
**Events:**

- Quantum Matters in Materials Science (QMMS)
- Artificial Intelligence for Materials Science (AIMS)
- JARVIS-School

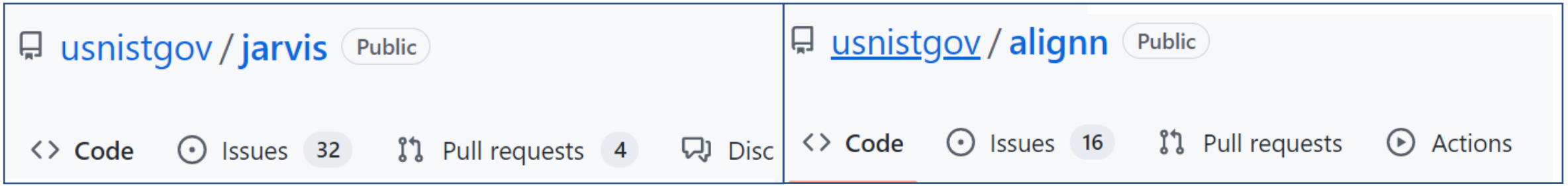



*User-comments:*

- *"There are many different theoretical levels on which you can approach the field. JARVIS is unusual in that it spans more levels than other databases."*
- *"A pure gold-mine for the data-quality effort…"*
- *Thanks for your generous sharing. Your works inspire me a lot.*
- *"You guys are doing something really beneficial…"*
- *"I find JARVIS-DFT very useful for my research…"*


[Choudhary et al., npj Computational Materials 6, 173 (2020).]

# Tools


usnistgov / jarvis
Public
Code
Issues 32
Pull requests 4
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usnistgov / alignn
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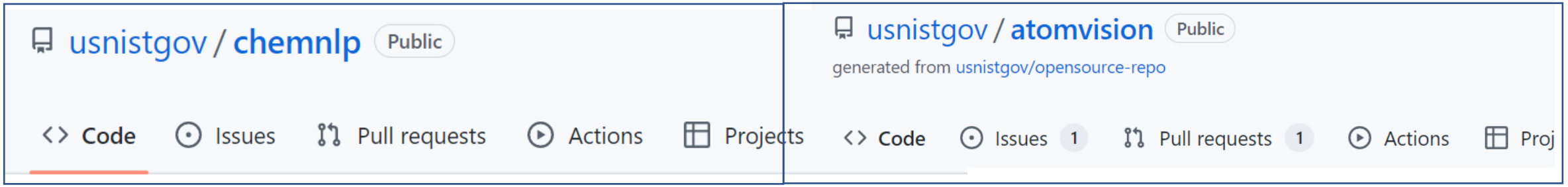
Code
Issues 16
Pull requests
Actions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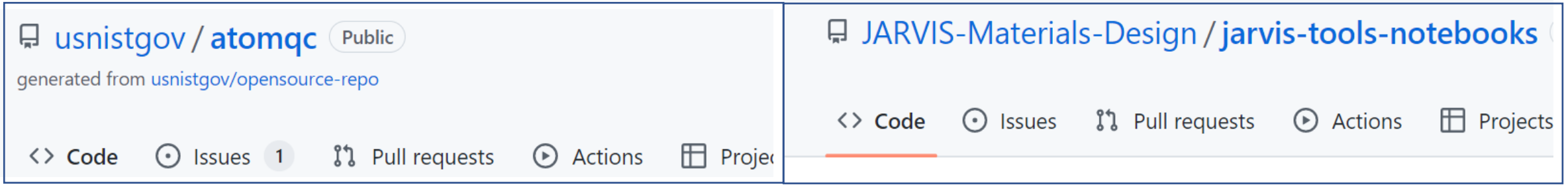
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Actions


JARVIS-Materials-Design / jarvis-tools-notebooks
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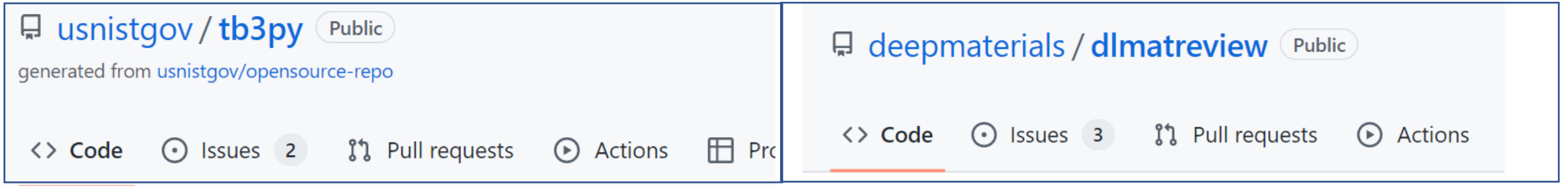
Issues
Pull requests
Actions
Projects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Code
Issues 2
Pull requests
Actions


deepmaterials / dlmatreview
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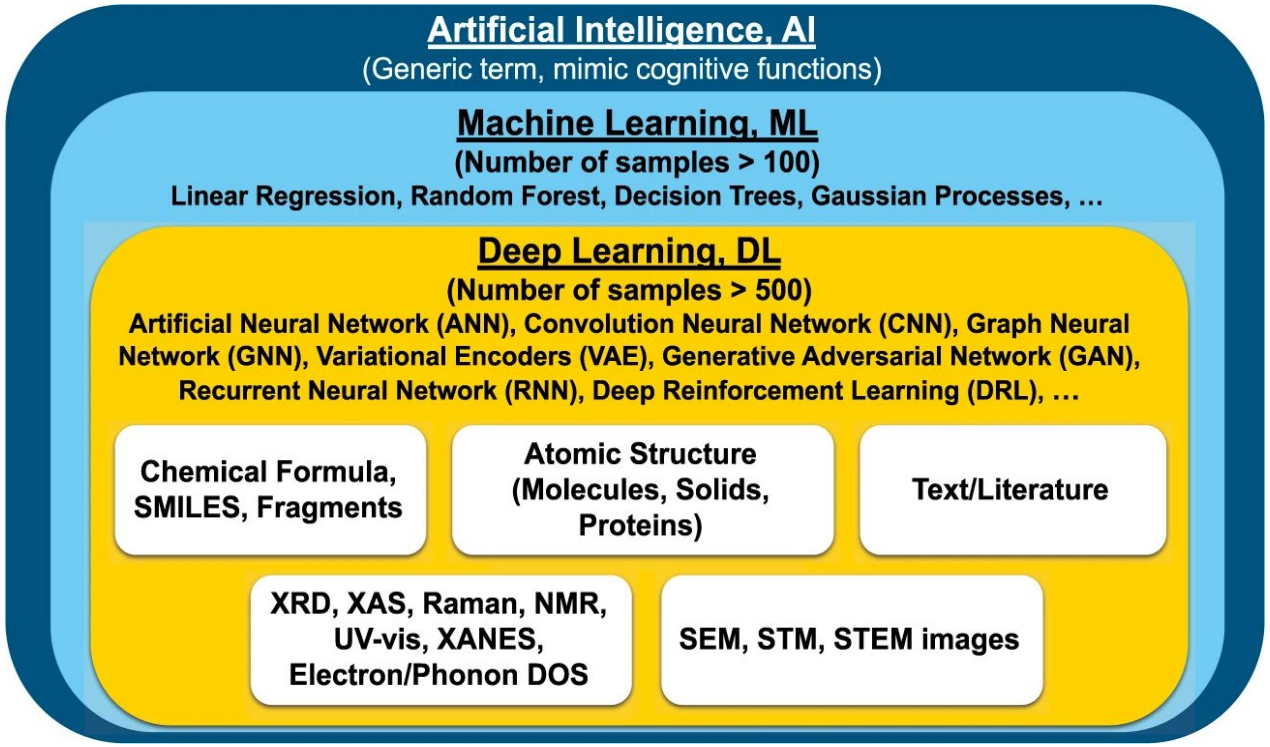
Code
Issues 3
Pull requests
Actions

# Introduction: deep learning for materials

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Review Article | Open Access | Published: 05 April 2022

## Recent advances and applications of deep learning methods in materials science

Kamal Choudhary, Brian DeCost, Chi Chen, Anubhav Jain, Francesca Tavazza, Ryan Cohn, Cheol Woo Park, Alok Choudhary, Ankit Agrawal, Simon J. L. Billinge, Elizabeth Holm, Shyue Ping Ong & Chris Wolverton

*npj Computational Materials* **8**, Article number: 59 (2022) | Cite this article

# ALIGNN

## Atomistic Line Graph Neural Network

## https://github.com/usnistgov/alignn

usnistgov / alignn Public

Notifications | Fork 50 | Star 102

Code | Issues 18 | Pull requests 2 | Actions | Projects | Security | Insights

main | 22 branches | 30 tags | Go to file | Code

knc6 Merge pull request #87 from usnistgov/develop ... 736ec73 on Jan 10 450 commits

| | | |
|---|---|---|
| .github | FIX IGNITE. | 3 months ago |
| alignn | Add package_data in setup.py for loading config and model ... | last month |
| .gitignore | Modified gitignore | 6 months ago |
| .pre-commit-config.yaml | reduce range for momentum annealing | 2 years ago |
| LICENSE.rst | Update and rename LICENSE to LICENSE.rst | 2 years ago |
| README.md | Added supercon model, added FF dataset for elements from... | last month |
| pyproject.toml | fix newline in pyproject.toml | 2 years ago |
| setup.py | Add package_data in setup.py for loading config and model ... | last month |

### About

Atomistic Line Graph Neural Network

jarvis.nist.gov/jalignn/

Readme

View license

102 stars

10 watching

50 forks

### Releases 30

v2023.01.10 Latest

on Jan 10

# Notebook

github.com/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/Training_ALIGNN_model_example.ipynb

Code | Blame | 2568 lines (2568 loc) · 128 KB

JARVIS-Materials-Design / jarvis-tools-notebooks

Code | Issues | Pull requests | Actions | Projects

Open in Colab

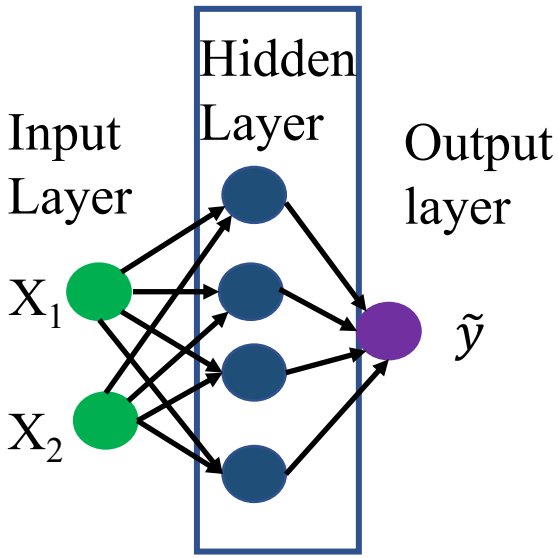
## Table of contents



In [1]:
```
!pip install alignn
```

# From ANNs to Graph Convolution Networks

## Standard NN




1) Forward propagation

$$z^{[l]} = W^{[l]} a^{[l-1]} + b^{[l]}$$

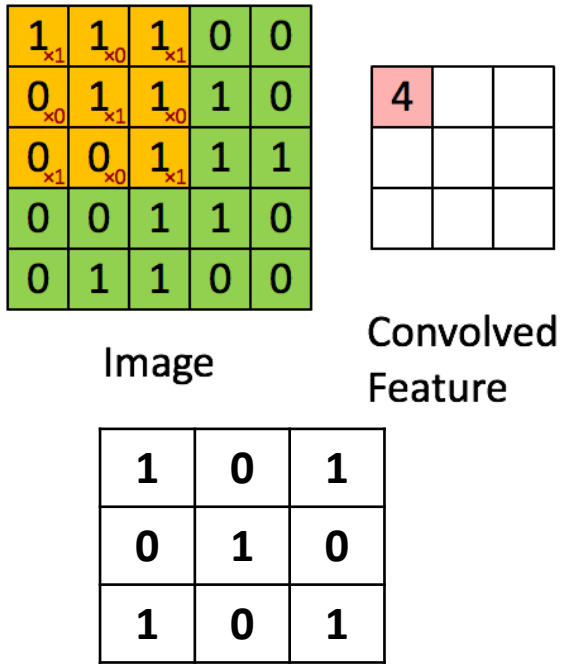
$$a^{[1]} = \sigma(z^{[l]}); \quad a^{[0]} = X$$

2) $Cost, J(W, b) = f(y - \tilde{y})$

3) Gradient descent (∇J):
minimize cost with W,b

4) Backpropagation:
chain rule to get, $\frac{\partial J}{\partial W}$

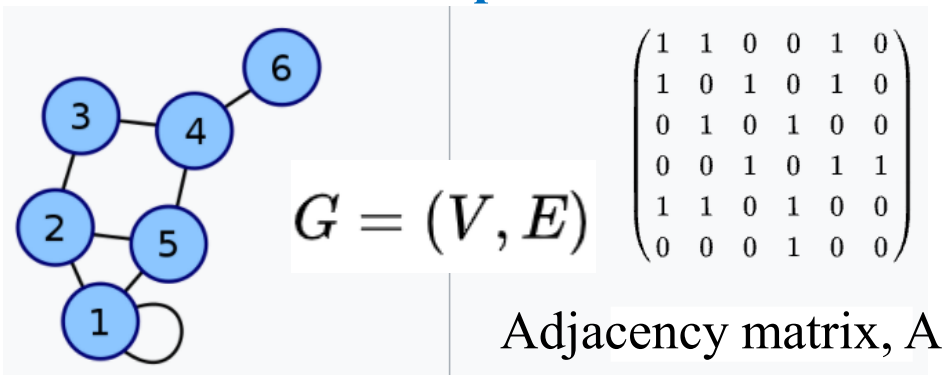
## ConvolutionNN




| | | |
|---|---|---|
| 1 | 0 | 1 |
| 0 | 1 | 0 |
| 1 | 0 | 1 |

1) Convolution:
element-wise multiplication & sum
2) Pool: Max, Average, Sum
3) Fully Connected: Standard NN
Shared weights (Learnable filters), regularized version of NNs

## GraphConvNN




Types: un/weighted, un/directed, line, Hetero/Homogenous, Multigraph

1) Adjacency matrix, N x N (N: #nodes),
2) D: degree of node
3) Update node representation using message passing, GPU efficient
4) Update equation is local, neighborhood of a node only, independent of graph size

$$\hat{A} = \tilde{D}^{-\frac{1}{2}} A \tilde{D}^{-\frac{1}{2}} \quad H^{l+1} = \sigma\left(W \hat{A} H^{l}\right)$$

$$h_i^{\ell+1} = f(h_i^{\ell}, \{h_j^{\ell}\}_{j \in \mathcal{N}_i})$$

arXiv.org > cs > arXiv:2003.00982

Search...

He

**Computer Science > Machine Learning**

*[Submitted on 2 Mar 2020 (v1), last revised 3 Jul 2020 (this version, v3)]*

# Benchmarking Graph Neural Networks

Vijay Prakash Dwivedi, Chaitanya K. Joshi, Thomas Laurent, Yoshua Bengio, Xavier Bresson

Graph neural networks (GNNs) have become the standard toolkit for analyzing and learning from data on graphs. As the field grows, it becomes critical to identify key architectures and validate new ideas that generalize to larger, more complex datasets. Unfortunately, it has been increasingly difficult to gauge the effectiveness of new models in the absence of a standardized benchmark with consistent experimental settings. In this paper, we introduce a reproducible GNN benchmarking framework, with the facility for researchers to add new models conveniently for arbitrary datasets. W demonstrate the usefulness of our framework by presenting a principled investigation into the recent Weisfeiler-Lehman GNNs (WL-GNNs) compared to message passing-based graph convolution networks (GCNs) for a variety of graph tasks, i.e. graph regression/classification and node/link prediction, with medium-scale datasets.

Comments: Benchmarking framework on GitHub at this https URL
Subjects: **Machine Learning (cs.LG)**; Machine Learning (stat.ML)
Cite as: arXiv:2003.00982 **[cs.LG]**
(or arXiv:2003.00982v3 **[cs.LG]** for this version)

graphdeeplearning / benchmarking-gnns Public

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master 6 branches 0 tags Go to file Add file Code

vijaydwivedi75 Update leaderboard 62c32cc on Jul 28 36 commits

| | | |
|---|---|---|
| configs | LapPE (#32) | 15 months ago |
| data | minor code clean | 11 months ago |
| docs | Update leaderboard | 2 months ago |
| layers | inbuilt reduce funcs (#55) | 10 months ago |

About

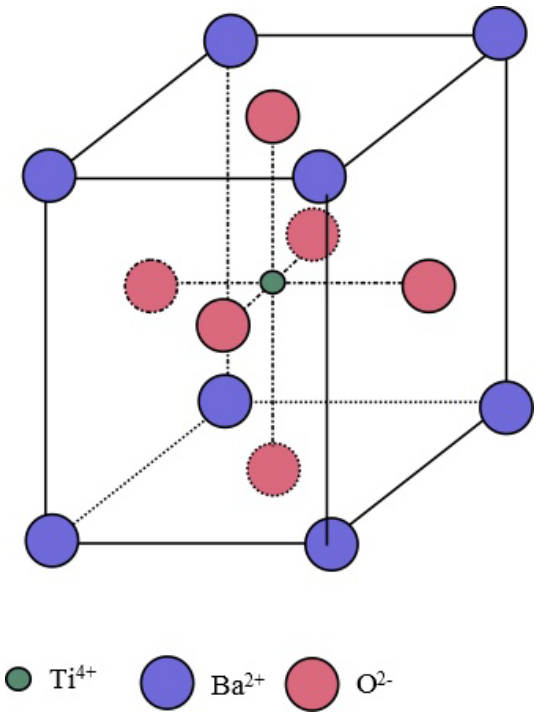
Repository for benchmarking graph neural networks

arxiv.org/abs/2003.00982

deep-learning pytorch benchmark-framework graph-neural-networks graph-representation-learning dgl

# Graph Convolution Networks for Materials Scientists

Consider $BaTiO_3$: start with $n_{input}$ -dimensional atom feature vectors $h_{Ti}$ $h_{Ba}$ $h_O$




The local environment of Ti can be modeled as:

$$h'_{Ti} = 6f(h_{Ti}, h_O, r_{TiO}) + 8f(h_{Ti}, h_{Ba}, r_{TiBa})$$

In GCNs, f is parameterized by one or more neural network layers

*e.g. edge-gated graph convolution:* arxiv:1711.07553

$$f(h_i, h_j, r_{ij}) = \phi_{gate}([h_i; h_j; \phi_{rbf}(r_{ij})]) \odot \phi_{pair}([h_i; h_j])$$

**Graph embedding** transform and encode the data structure in high dimensional and non-Euclidean feature space to a low dimensional space

$\odot$ Elementwise multiplication

$[a;\ b]$ denotes concatenation

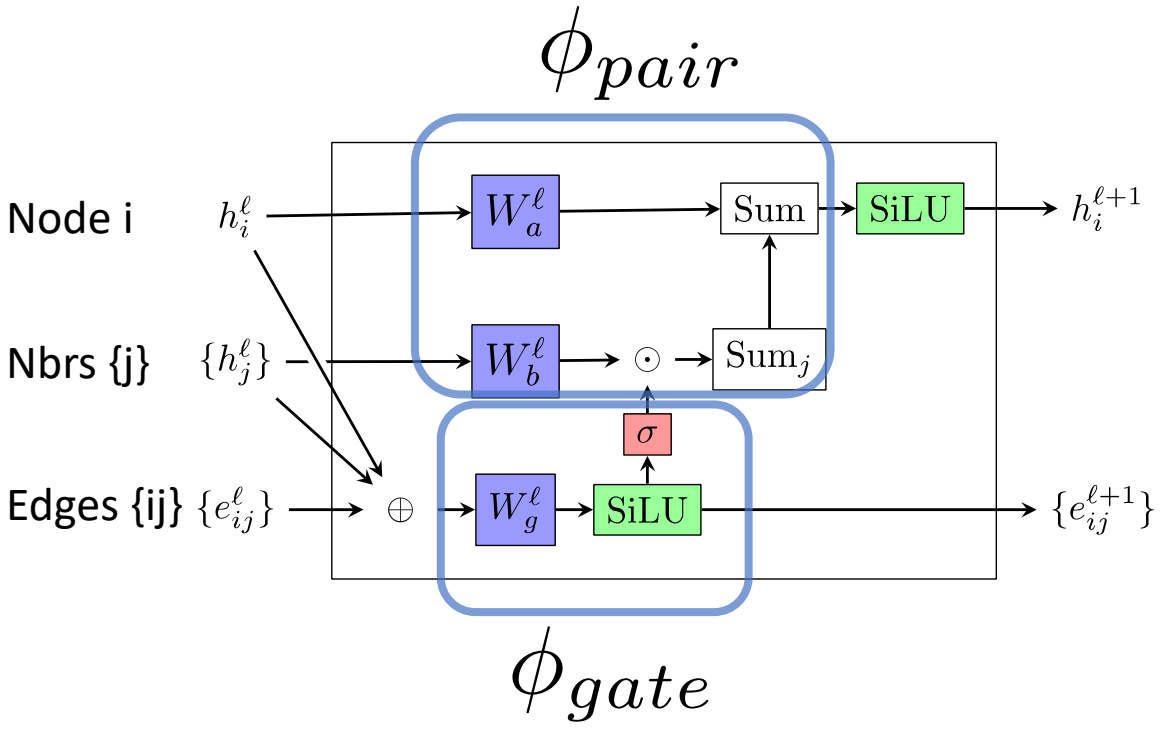
$\phi_{pair}$ is a neural network modeling pairwise atom interactions

$\phi_{gate}$ is a neural network modeling the importance of $\phi_{pair}$ output channels as a function of bond character

GCNs implicitly represent multi-body interactions by composing multiple layers

# Edge-gated Graph Convolution Layer

$$\phi_{gate}([h_i; h_j; \phi_{rbf}(r_{ij})]) \odot \phi_{pair}([h_i; h_j])$$




For computational efficiency, the $\phi_{pair}$ parameters are split into two separate matrices
see [https://docs.dgl.ai/guide/message-efficient.html](https://docs.dgl.ai/guide/message-efficient.html)

adapted from:

graphdeeplearning / benchmarking-gnns Public

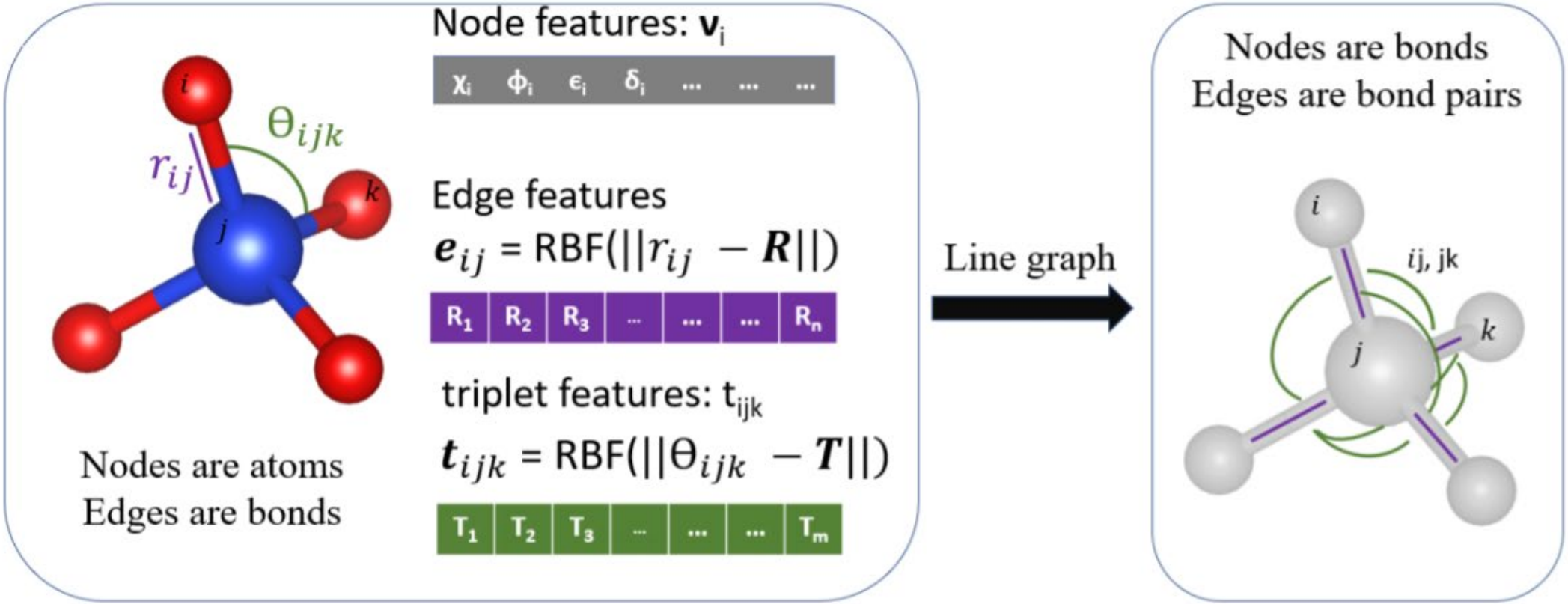
<> Code | Issues 3 | Pull requests | Discussions

```python
def forward(
    self,
    g: dgl.DGLGraph,
    node_feats: torch.Tensor,
    edge_feats: torch.Tensor,
) -> torch.Tensor:
    """Edge-gated graph convolution.
    h_i^l+1 = SiLU(U h_i + sum_{j->i} eta_{ij} ⊙ V h_j)
    """
    g = g.local_var()

    # compute edge updates, equivalent to:
    # Softplus(Linear(u || v || e))
    g.ndata["e_src"] = self.src_gate(node_feats)
    g.ndata["e_dst"] = self.dst_gate(node_feats)
    g.apply_edges(fn.u_add_v("e_src", "e_dst", "e_nodes"))
    m = g.edata.pop("e_nodes") + self.edge_gate(edge_feats)

    g.edata["sigma"] = torch.sigmoid(m)
    g.ndata["Bh"] = self.dst_update(node_feats)
    g.update_all(
        fn.u_mul_e("Bh", "sigma", "m"), fn.sum("m", "sum_sigma_h")
    )
    g.update_all(fn.copy_e("sigma", "m"), fn.sum("m", "sum_sigma"))
    g.ndata["h"] = g.ndata["sum_sigma_h"] / (g.ndata["sum_sigma"] + 1e-6)
    x = self.src_update(node_feats) + g.ndata.pop("h")

    # node and edge updates
    x = F.silu(self.bn_nodes(x))
    y = F.silu(self.bn_edges(m))
```

DEEP GRAPH LIBRARY

# Line Graph

**Explicitly represent pairwise and triplet (bond angle) interactions using line graph**
**Possible to extend for n-body, *e.g.* line graph of line graph**

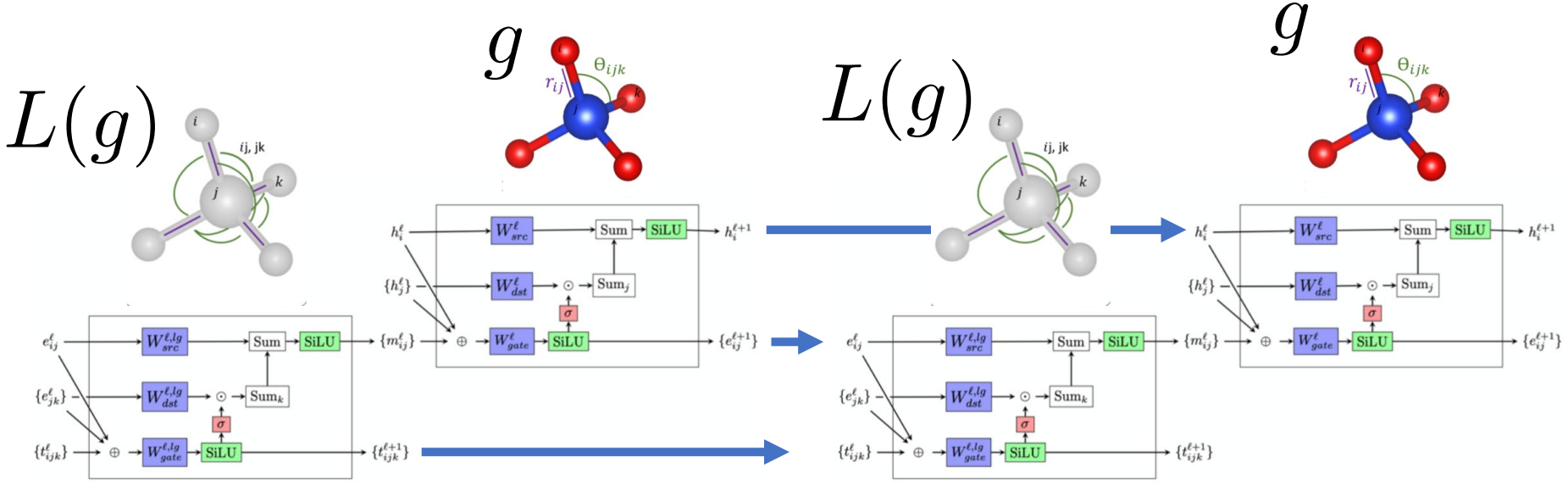



**nisaba.nist.gov** Tesla V100

# ALIGNN Model

Compose multiple ALIGNN and EdgeGatedGCN layers: learnable local atom environment representation
Global crystal representation: Feature-wise average across atoms in the crystal
Final property regression model: linear model for regression, logistic regression for classification

Initial atom, bond, angle features




Feature-wise sum across atoms

Property prediction

```python
@staticmethod
def atom_dgl_multigraph(
    atoms=None,
    neighbor_strategy="k-nearest",
    cutoff=8.0,
    max_neighbors=12,
    atom_features="cgcnn",
    max_attempts=3,
    id: Optional[str] = None,
    compute_line_graph: bool = True,
    use_canonize: bool = False,
):
    """Obtain a DGLGraph for Atoms object
    if neighbor_strategy == "k-nearest":
        edges = nearest_neighbor_edges(
            atoms=atoms,
            cutoff=cutoff,
            max_neighbors=max_neighbors,
            id=id,
            use_canonize=use_canonize,
        )
    else:
        raise ValueError("Not implemented
    # elif neighbor_strategy == "voronoi"
    #     edges = voronoi_edges(structure)
```

```python
class ALIGNN(nn.Module):
    """Atomistic Line graph network.

    Chain alternating gated graph convolution updates on crystal graph
    and atomistic line graph.
    """

    def __init__(self, config: ALIGNNConfig = ALIGNNConfig(name="alignn'
        """Initialize class with number of input features, conv layers."
        super().__init__()
        print(config)
        self.classification = config.classification

        self.atom_embedding = MLPLayer(
            config.atom_input_features, config.hidden_features
        )

        self.edge_embedding = nn.Sequential(
            RBFExpansion(
                vmin=0,
                vmax=8.0,
                bins=config.edge_input_features,
            ),
            MLPLayer(config.edge_input_features, config.embedding_featu
            MLPLayer(config.embedding_features, config.hidden_features),
        )
        self.angle_embedding = nn.Sequential(
            RBFExpansion(
                vmin=-1,
                vmax=1.0,
                bins=config.triplet_input_features,
            ),
            MLPLayer(config.triplet_input_features, config.embedding_fea
            MLPLayer(config.embedding_features, config.hidden_features),
        )
```

```python
self.alignn_layers = nn.ModuleList(
    [
        ALIGNNConv(
            config.hidden_features,
            config.hidden_features,
        )
        for idx in range(config.alignn_layers)
    ]
)
self.gcn_layers = nn.ModuleList(
    [
        EdgeGatedGraphConv(
            config.hidden_features, config.hidden_features
        )
        for idx in range(config.gcn_layers)
    ]
)

self.readout = AvgPooling()

if self.classification:
    self.fc = nn.Linear(config.hidden_features, 2)
    self.softmax = nn.LogSoftmax(dim=1)
else:
    self.fc = nn.Linear(config.hidden_features, config.output_features)
self.link = None
self.link_name = config.link
if config.link == "identity":
    self.link = lambda x: x
elif config.link == "log":
    self.link = torch.exp
    avg_gap = 0.7  # magic number -- average bandgap in dft_3d
    self.fc.bias.data = torch.tensor(
        np.log(avg_gap), dtype=torch.float
    )
elif config.link == "logit":
    self.link = torch.sigmoid
```

# Performance on the Materials Project Dataset

Trained on 69239 materials (DFT data)

#Epochs: 300
Batch_size: 64

**Table 1 Performance on the materials project dataset.**

| Prop | Unit | MAD | CFID | CGCNN | MEGNet | SchNet | ALIGNN | MAD:MAE |
|---|---|---|---|---|---|---|---|---|
| $E_f$ | eV/atom | 0.93 | 0.104 | 0.039 | 0.028 | 0.035 | 0.0221 | 42.08 |
| $E_g$ | eV | 1.35 | 0.434 | 0.388 | 0.33 | - | 0.218 | 6.19 |

- **~44 % improvement by ALIGNN with similar/better training speed**
- **Similar performance enhancement on QM9 molecule dataset**
- **Also available on MatBench: https://matbench.materialsproject.org**

# Performance on the JARVIS-DFT Dataset

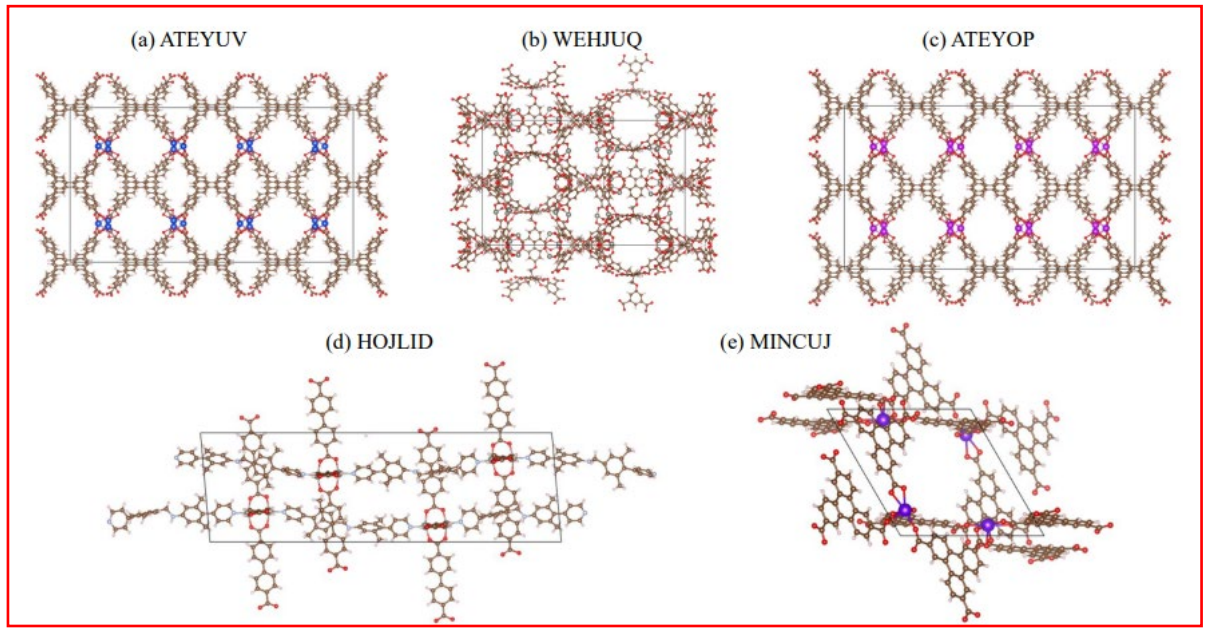
| Property | Units | MAD | CFID | CGCNN | ALIGNN | MAD: MAE |
|---|---|---|---|---|---|---|
| Formation energy | eV(atom)$^{-1}$ | 0.86 | 0.14 | 0.063 | 0.033 | 26.06 |
| Bandgap (OPT) | eV | 0.99 | 0.30 | 0.20 | 0.14 | 7.07 |
| Total energy | eV(atom)$^{-1}$ | 1.78 | 0.24 | 0.078 | 0.037 | 48.11 |
| Ehull | eV | 1.14 | 0.22 | 0.17 | 0.076 | 15.00 |
| Bandgap (MBJ) | eV | 1.79 | 0.53 | 0.41 | 0.31 | 5.77 |
| Kv | GPa | 52.80 | 14.12 | 14.47 | 10.40 | 5.08 |
| Gv | GPa | 27.16 | 11.98 | 11.75 | 9.48 | 2.86 |
| Mag. mom | μB | 1.27 | 0.45 | 0.37 | 0.26 | 4.88 |
| SLME (%) | No unit | 10.93 | 6.22 | 5.66 | 4.52 | 2.42 |
| Spillage | No unit | 0.52 | 0.39 | 0.40 | 0.35 | 1.49 |
| Kpoint-length | Å | 17.88 | 9.68 | 10.60 | 9.51 | 1.88 |
| Plane-wave cutoff | eV | 260.4 | 139.4 | 151.0 | 133.8 | 1.95 |
| $\epsilon_x$ (OPT) | No unit | 57.40 | 24.83 | 27.17 | 20.40 | 2.81 |
| $\epsilon_y$ (OPT) | No unit | 57.54 | 25.03 | 26.62 | 19.99 | 2.88 |
| $\epsilon_z$ (OPT) | No unit | 56.03 | 24.77 | 25.69 | 19.57 | 2.86 |

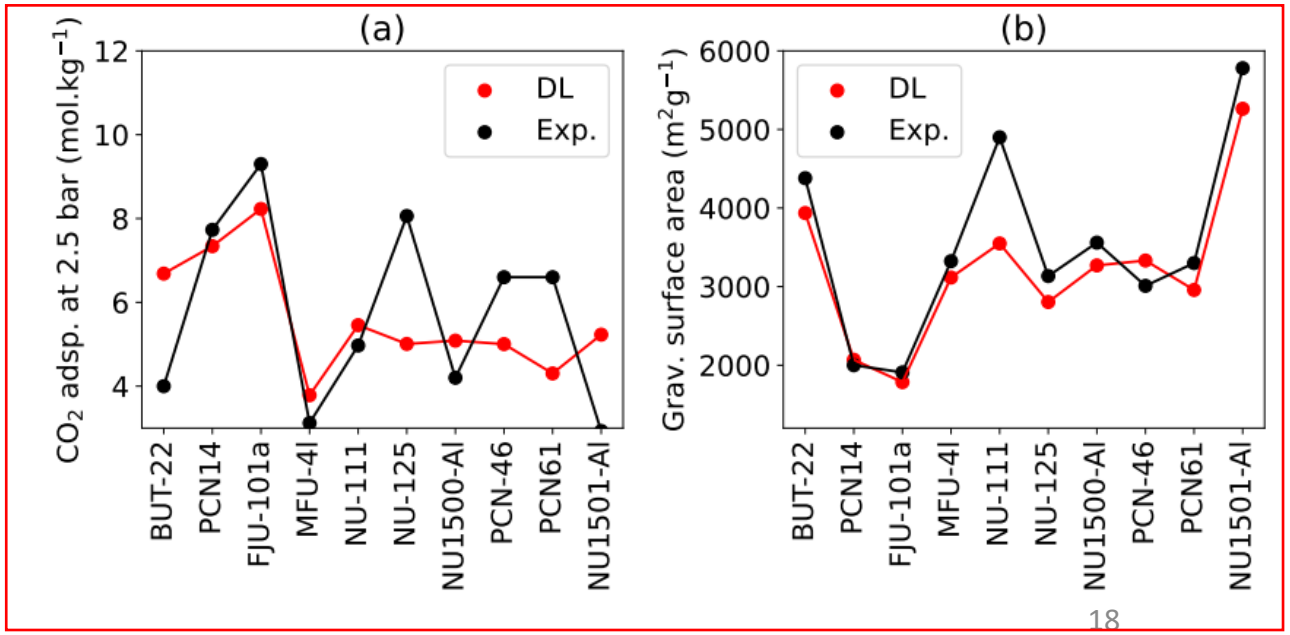
Trained on ~55k materials

- Total energy, Formation energy , Ehull
- Bandgap (OPT), Bandgap (MBJ)
- Kv, Gv
- Mag. mom
- ϵx (OPT/MBJ), ϵy (OPT), ϵz (OPT), ϵ (DFPT:elec+ionic)
- Max. piezo. stress coeff (eij)
- Solar-SLME (%)
- Topological-Spillage
- 2D-Exfo. energy
- Kpoint-length
- Plane-wave cutoff
- Max. Electric field gradient
- avg. $m_e$, avg. $m_h$
- n-Seebeck, n-PF, p-Seebeck, p-PF

# $CO_2$ Isotherms: AI for Climate Change

DL model for predicting $CO_2$ adsorption in MOFs (using hMOF GCMC data)


Choudhary et al., Computational Materials Science 210, 111388 (2022)

# BCS Superconductors & E-Ph coupling

**Superconductors**: Materials to conduct electricity without energy loss when they are cooled below a critical temperature, Tc

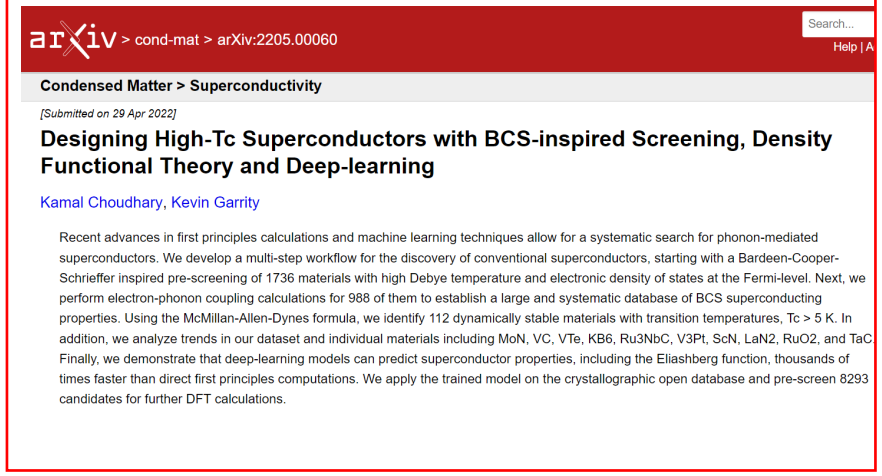
**$MgB_2$** ($T_c$ = 39 K): Highest Tc ambient condition conventional superconductor

$$T_c = K\Theta_D \exp\left(-\frac{1}{N(0)V}\right)$$

Debye Temp

DOS at $E_{Fermi}$

https://arxiv.org/abs/2205.00060



arXiv > cond-mat > arXiv:2205.00060

Search... Help | A

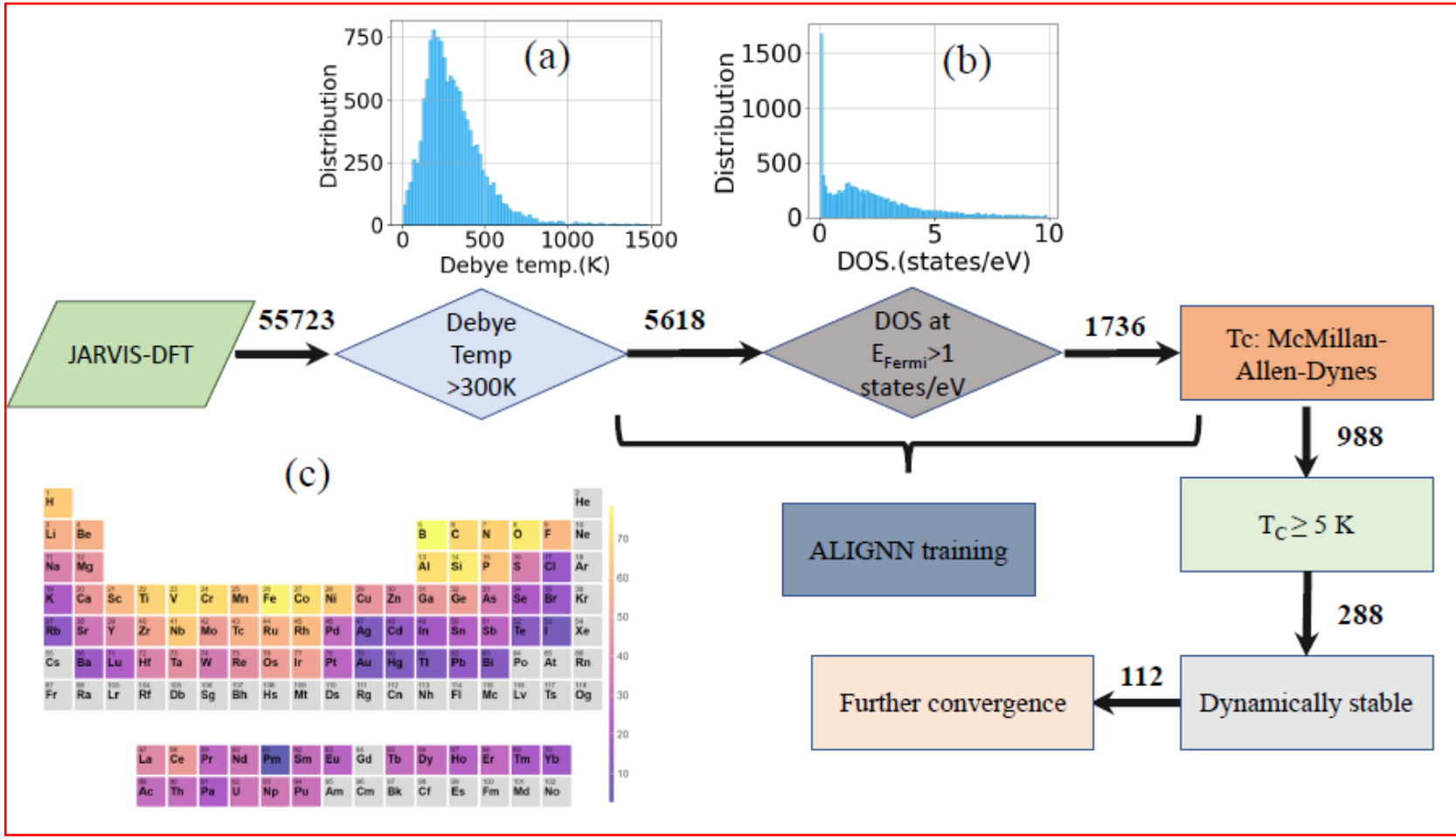
Condensed Matter > Superconductivity

[Submitted on 29 Apr 2022]

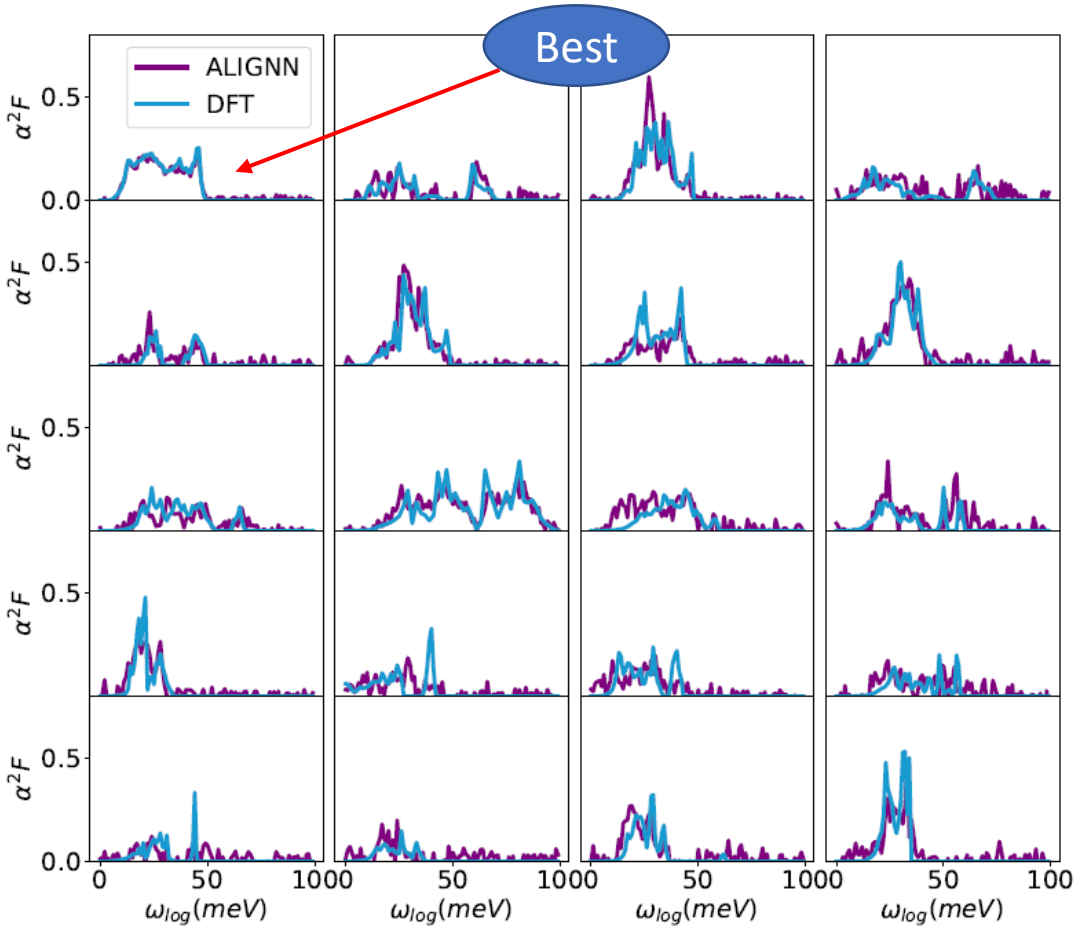
**Designing High-Tc Superconductors with BCS-inspired Screening, Density Functional Theory and Deep-learning**

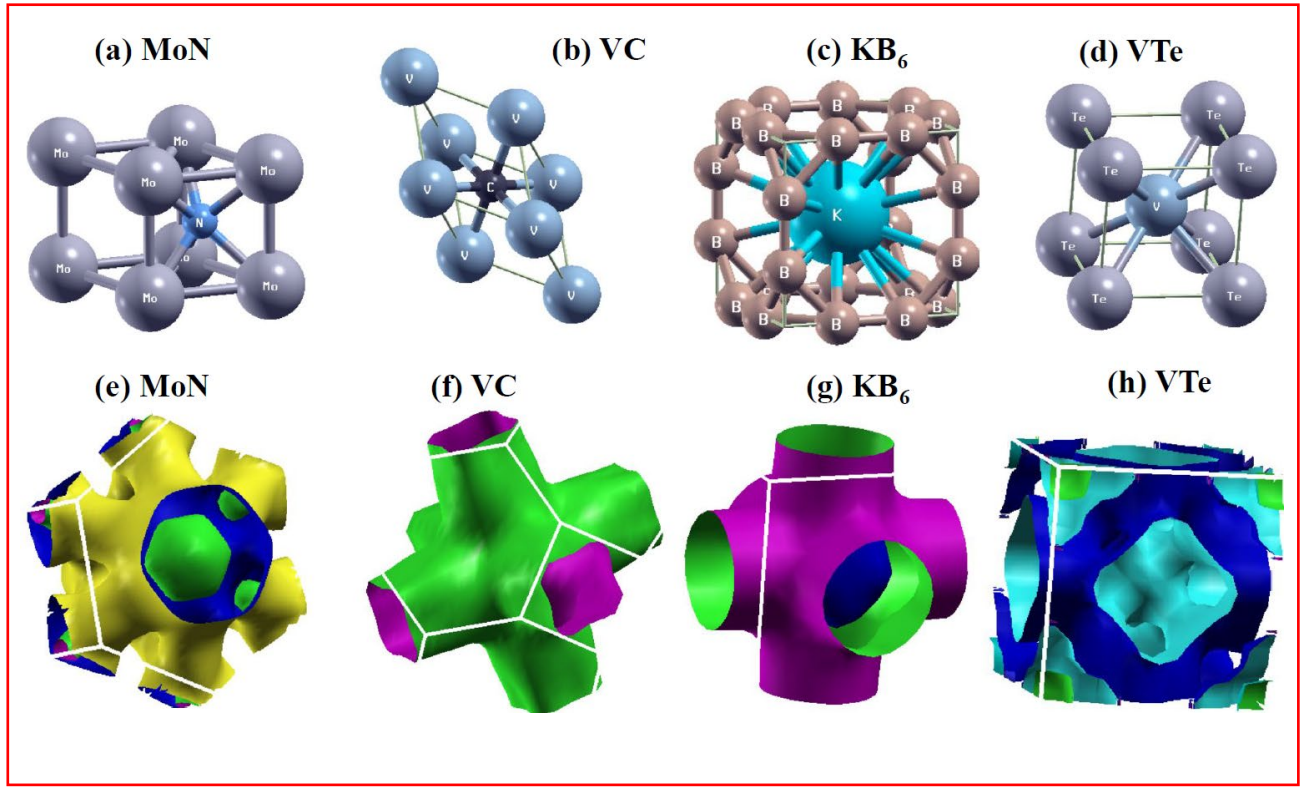
Kamal Choudhary, Kevin Garrity

Recent advances in first principles calculations and machine learning techniques allow for a systematic search for phonon-mediated superconductors. We develop a multi-step workflow for the discovery of conventional superconductors, starting with a Bardeen-Cooper-Schrieffer inspired pre-screening of 1736 materials with high Debye temperature and electronic density of states at the Fermi-level. Next, we perform electron-phonon coupling calculations for 988 of them to establish a large and systematic database of BCS superconducting properties. Using the McMillan-Allen-Dynes formula, we identify 112 dynamically stable materials with transition temperatures, Tc > 5 K. In addition, we analyze trends in our dataset and individual materials including MoN, VC, VTe, KB6, Ru3NbC, V3Pt, ScN, LaN2, RuO2, and TaC. Finally, we demonstrate that deep-learning models can predict superconductor properties, including the Eliashberg function, thousands of times faster than direct first principles computations. We apply the trained model on the crystallographic open database and pre-screen 8293 candidates for further DFT calculations.



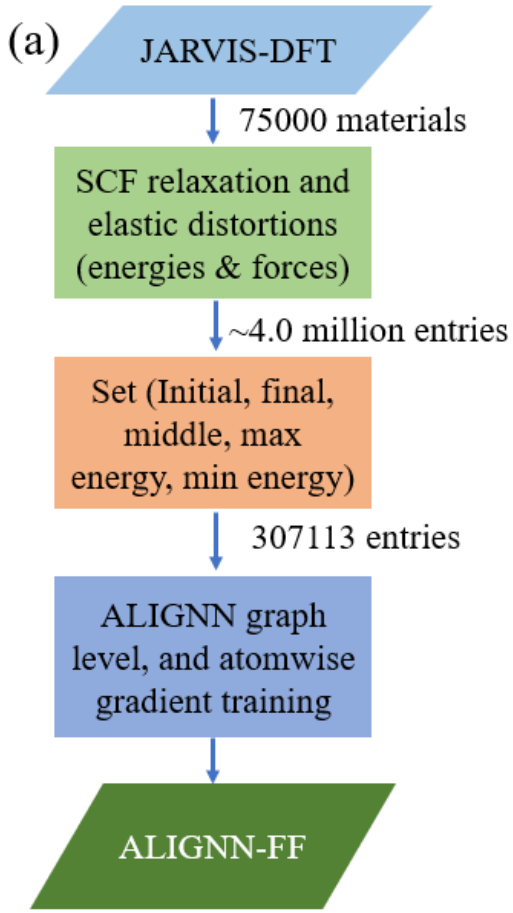
# BCS Superconductors

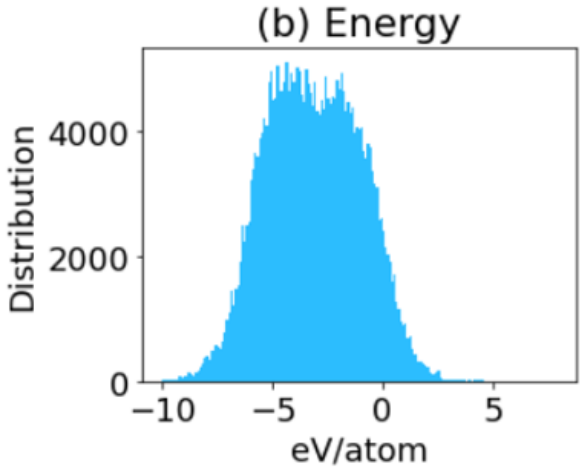


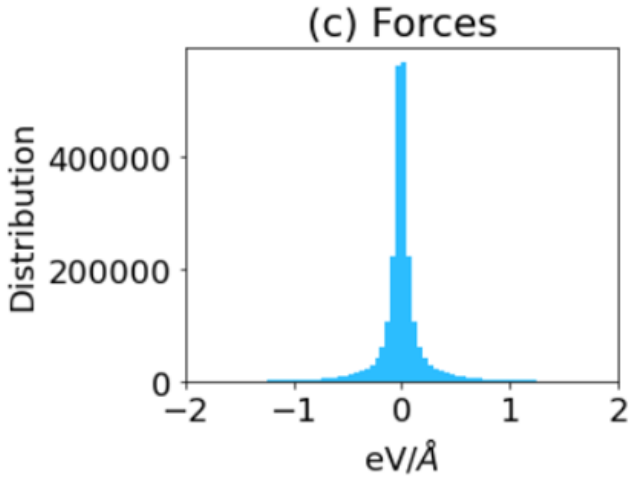



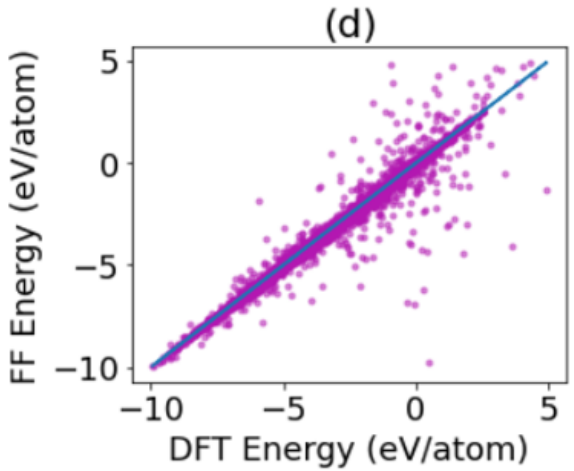

- Prediction on 10 % test data
- 8293 out of 431778 materials in COD as superconductors
- First predicting Eliashberg function, then Tc → 6 % improvement
- ALIGNN for both scalar and spectral learning

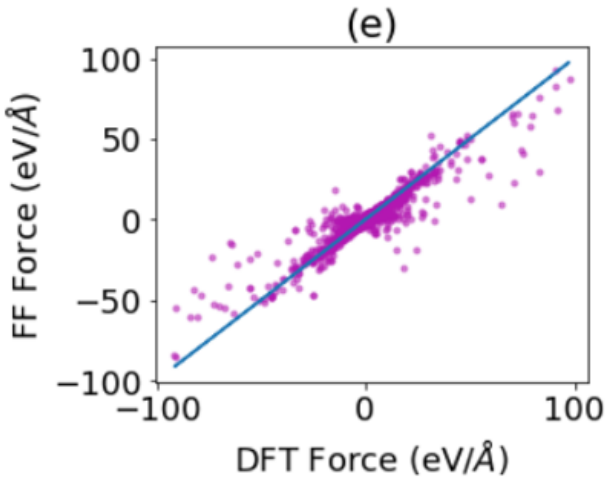
# Unified GNN Force-field




Simulate any combination of 89 elements from the periodic table

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Cite this: DOI: 10.1039/d2dd00096b

**Unified graph neural network force-field for the periodic table: solid state applications**

Kamal Choudhary, [*ab] Brian DeCost, [c] Lily Major, [de] Keith Butler, [e] Jeyan Thiyagalingam [e] and Francesca Tavazza [c]

| Weight | MAE-Energies (eV/atom) | MAE-Forces (eV/Å) |
|---|---|---|
| 0.1 | 0.034 | 0.092 |
| 0.5 | 0.044 | 0.089 |
| 1.0 | 0.051 | 0.088 |
| 5.0 | 0.082 | 0.054 |
| 10.0 | 0.086 | 0.047 |

$$l = \left|E^{DFT} - E^{GNN}\right| + w \sum_{i}^{N_{atoms}} \left|F_i^{DFT} - F_i^{GNN}\right|$$

# Unified GNN Force-field: Forces and stresses

Using $r_{ij}$, not $r_i$ for eqivariance:

$$m_i \frac{\mathrm{d}^2 r_i(t)}{\mathrm{d}t^2} = \sum_j F_{ij}(t) = -\sum_j \nabla_i U\left(r_{ij}(t)\right)$$

$$\sigma_{\alpha\beta} = -\frac{1}{V}\sum_i \sum_{i \neq j} F_{ij}^{\alpha} r_{ij}^{\beta} + m_i v_i^{\alpha} v_i^{\beta}$$

$$l = \left|E^{DFT} - E^{GNN}\right| + w \sum_i^{N_{atoms}} \left|F_i^{DFT} - F_i^{GNN}\right|$$

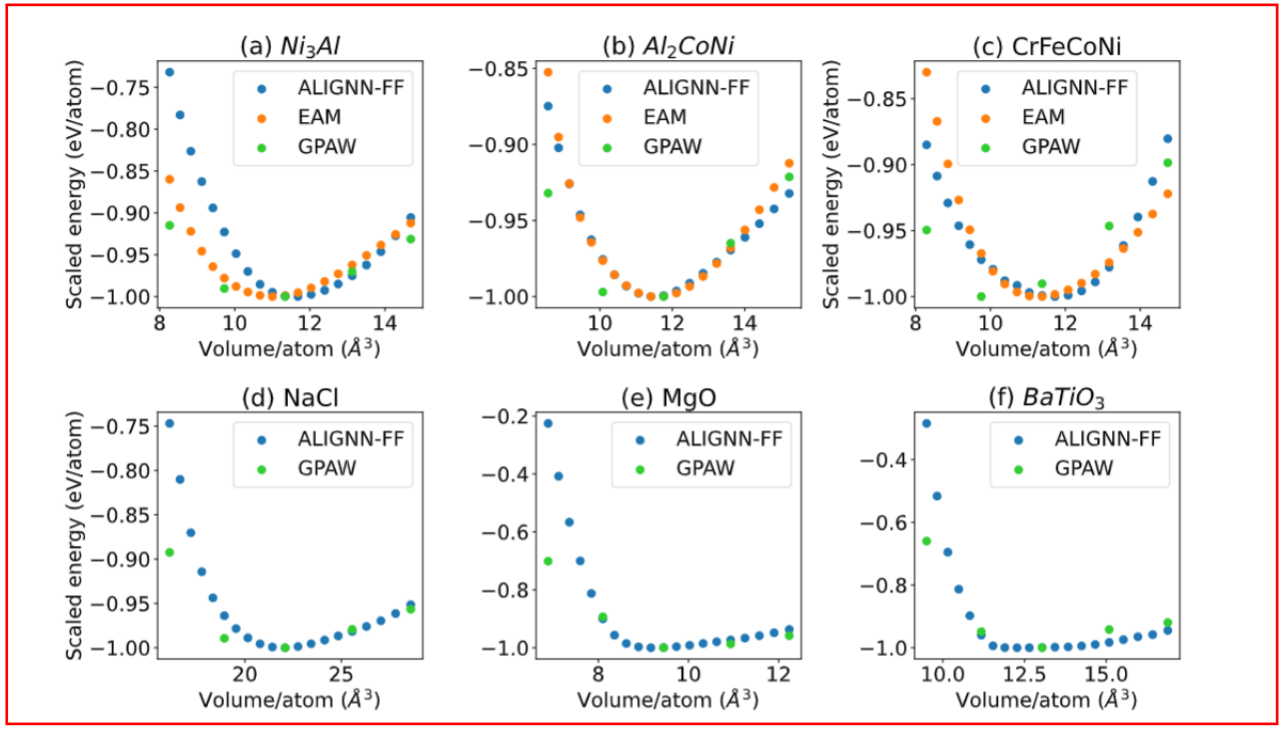
| Weight | MAE-Energies (eV/atom) | MAE-Forces (eV/Å |
|---|---|---|
| 0.1 | 0.034 | 0.092 |
| 0.5 | 0.044 | 0.089 |
| 1.0 | 0.051 | 0.088 |
| 5.0 | 0.082 | 0.054 |
| 10.0 | 0.086 | 0.047 |

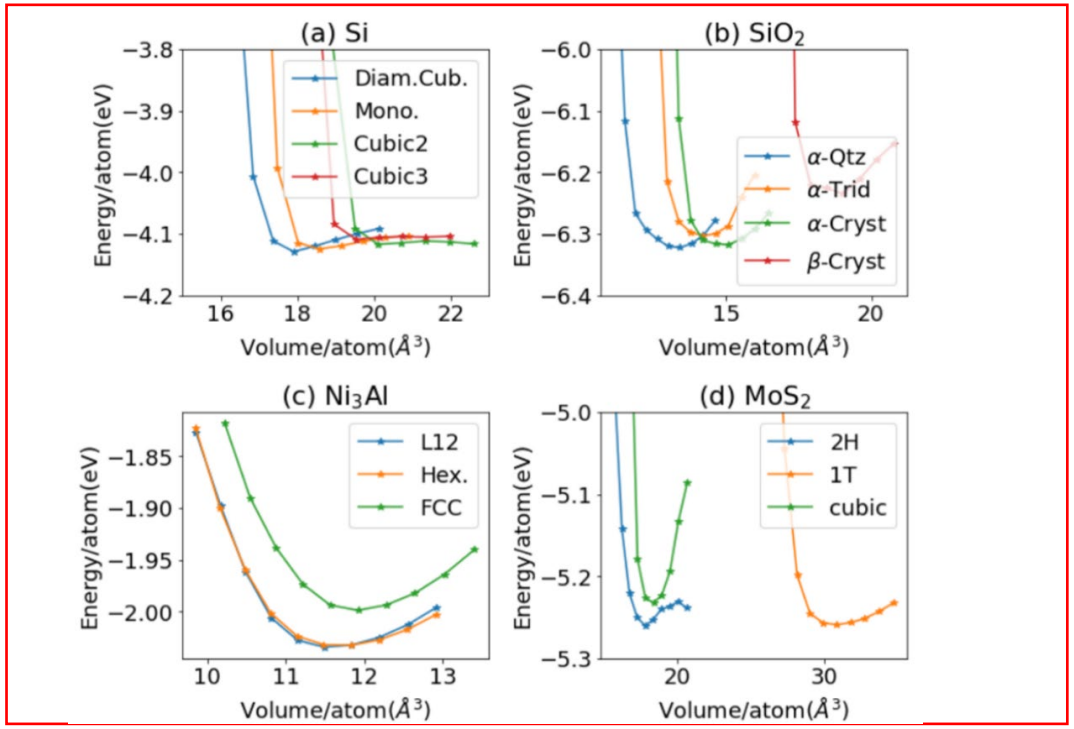
```
if self.config.calculate_gradient:
    create_graph = True

    dy = (
        self.config.grad_multiplier
        * grad(
            # tmp_out,
            out,
            r,
            grad_outputs=torch.ones_like(out),
            create_graph=create_graph,
            retain_graph=True,
        )[0]
    )
    g.edata["dy_dr"] = dy
    g.update_all(fn.copy_e("dy_dr", "m"), fn.sum("m", "gradient"))
    gradient = torch.squeeze(g.ndata["gradient"])
```

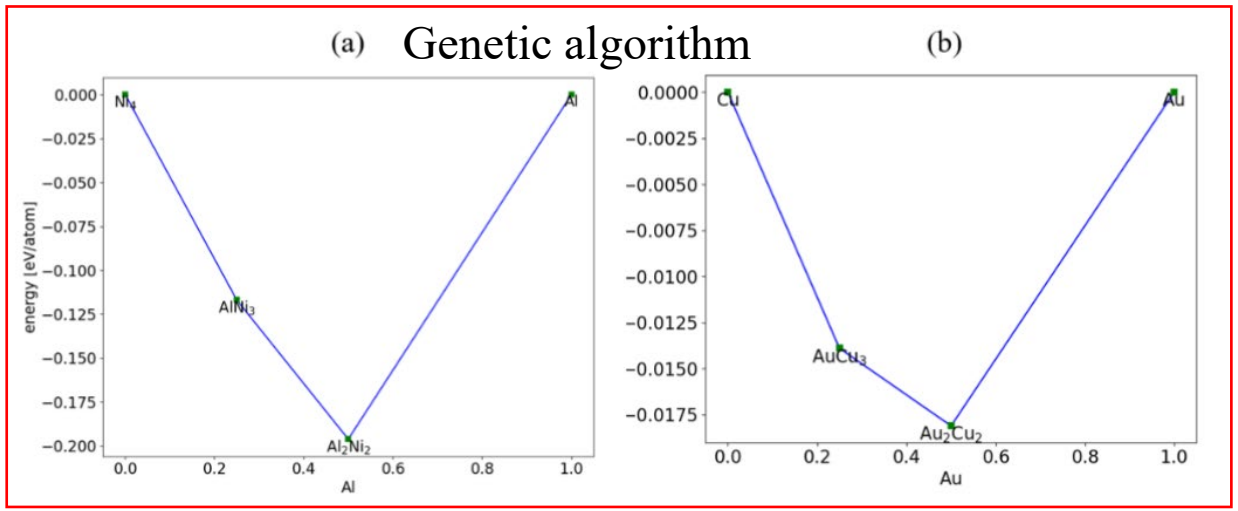
PyTorch AutoGrad function

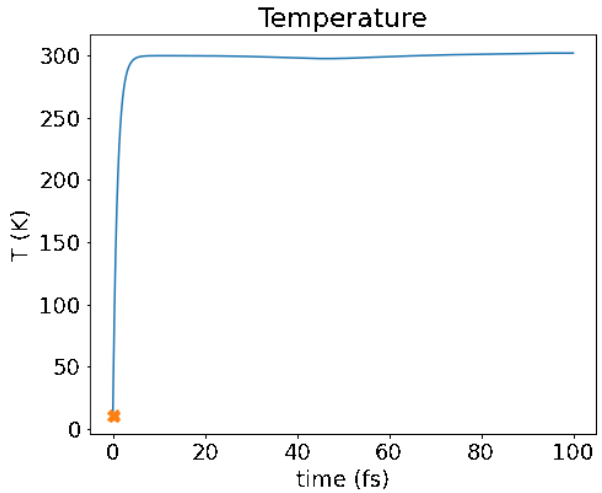
# Unified GNN Force-field

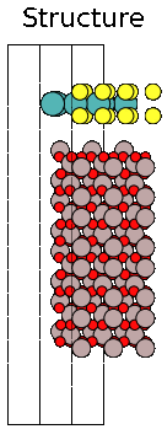
EV-curves




Example NVT : Interface of 2H-$MoS_2$(001)/ $Al_2O_3$(0001)

# Publications using ALIGNN

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## Atomistic Line Graph Neural Network for improved materials property predictions

Kamal Choudhary & Brian DeCost

*npj Computational Materials* **7**, Article number: 185 (2021) | Cite this article

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## Designing high-$T_C$ superconductors with BCS-inspired screening, density functional theory, and deep-learning

Kamal Choudhary & Kevin Garrity

*npj Computational Materials* **8**, Article number: 244 (2022) | Cite this article

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Computational Materials Science

Volume 210, July 2022, 111388

Full length article

## Graph neural network predictions of metal organic framework $CO_2$ adsorption properties

Kamal Choudhary [a b c], Taner Yildirim [d], Daniel W. Siderius [e], A. Gilad Kusne [f], Austin McDannald [f], Diana L. Ortiz-Montalvo [f]

## Prediction of the Electron Density of States for Crystalline Compounds with Atomistic Line Graph Neural Networks (ALIGNN)

Prathik R. Kaundinya, Kamal Choudhary & Surya R. Kalidindi

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## Unified graph neural network force-field for the periodic table: solid state applications

Kamal Choudhary, *[ab] Brian DeCost, [c] Lily Major, [de] Keith Butler, [e] Jeyan Thiyagalingam [e] and Francesca Tavazza [c]

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## Rapid prediction of phonon structure and properties using the atomistic line graph neural network (ALIGNN)

Ramya Gurunathan, Kamal Choudhary, and Francesca Tavazza

Phys. Rev. Materials **7**, 023803 – Published 24 February 2023

arXiv > cond-mat > arXiv:2205.08366

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**Condensed Matter > Materials Science**

*[Submitted on 17 May 2022]*

## A Deep-learning Model for Fast Prediction of Vacancy Formation in Diverse Materials

Kamal Choudhary, Bobby G. Sumpter

# AtomVision

## A deep learning framework for atomistic image data

usnistgov / atomvision Public

generated from usnistgov/opensource-repo

<> Code | Issues | Pull requests | Projects | Wiki | Security | Insights | Settings

master | 1 branch | 0 tags

knc6 Add github action.

| | |
|---|---|
| .github | Add github action |
| atomvision | Remove unnecessa |
| CODEMETA.yaml | Initial commit |
| LICENSE.md | Initial commit |
| README.md | Update README.m |
| setup.py | Fix requirements. |

README.md

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JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING

pubs.acs.org/jcim Article

**AtomVision: A Machine Vision Library for Atomistic Images**

Kamal Choudhary,* Ramya Gurunathan, Brian DeCost, and Adam Biacchi

Cite This: https://doi.org/10.1021/acs.jcim.2c01533 Read Online

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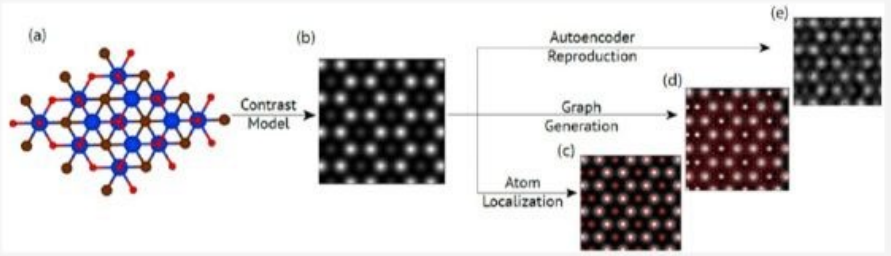

# Notebook

github.com/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/AtomVisionExample.ipynb

eated using Colaboratory

Code | Blame 1083 lines (1083 loc) · 685 KB

JARVIS-Materials-Design / jarvis-tools-notebooks

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## Example to run AtomVision

AtomVision is a deep learning package to perform various operations on image data including segmentation and classification of ima

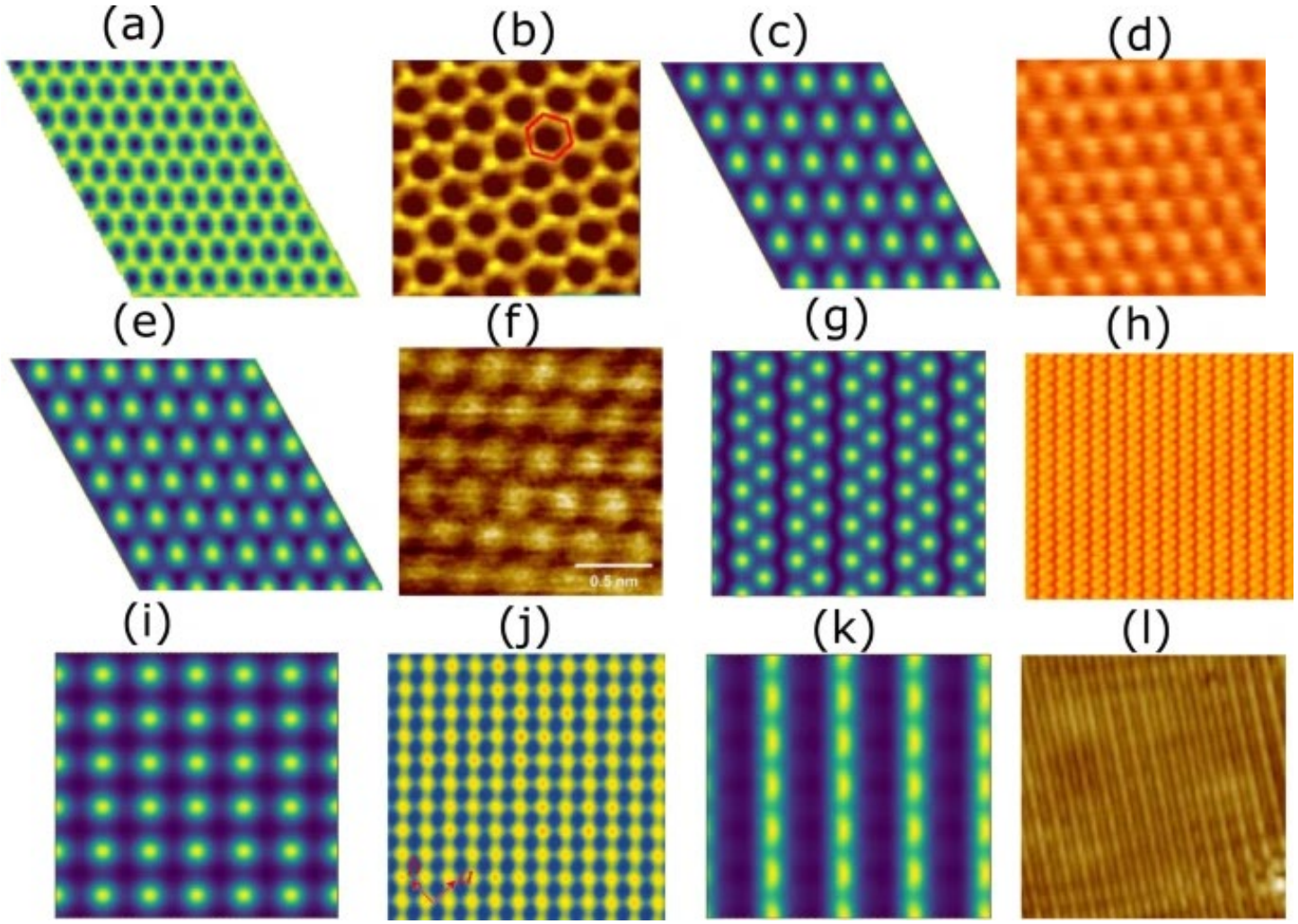
## Table of Contents

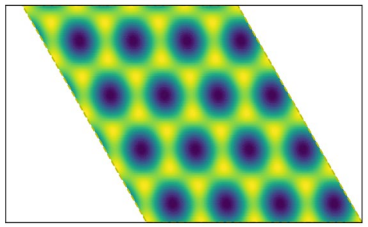


## Get the repository and install

In [1]:
```
pip install atomvision
```

# Scanning Tunneling Microscope Image



$$I_t \propto \rho(\boldsymbol{r}, E_F) \equiv \sum_\mu |\psi_\mu(\boldsymbol{r})|^2 \, \delta(\varepsilon_\mu - E_F)$$

Tersoff-Hamann Approach

nature › scientific data › data descriptors › article

Data Descriptor | Open Access | Published: 11 February 2021

**Computational scanning tunneling microscope image database**

Kamal Choudhary ✉, Kevin F. Garrity, Charles Camp, Sergei V. Kalinin, Rama Vasudevan, Maxim Ziatdinov & Francesca Tavazza

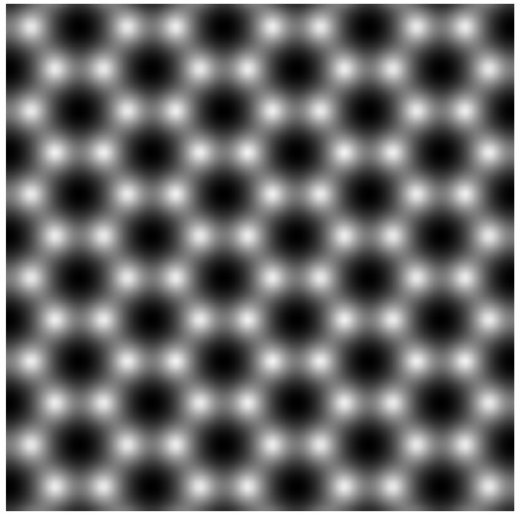
*Scientific Data* **8**, Article number: 57 (2021) | Cite this article

**1594** Accesses | **1** Citations | **4** Altmetric | Metrics

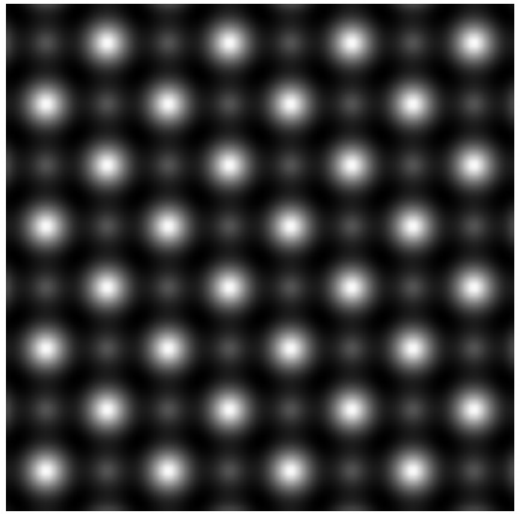
# Scanning Transmission Electron Microscope Image

Convolution approximation: accurate for **thin films** mainly (here 2D mats.)
Based on Rutherford scattering model

$$I(\boldsymbol{r}) = R(\boldsymbol{r}, Z) \otimes \mathrm{PSF}(\boldsymbol{r}) \qquad R(\boldsymbol{r}, Z) = \sum_{i=1}^{N} Z_i^{1.7} \delta(\boldsymbol{r} - \boldsymbol{r_i})$$



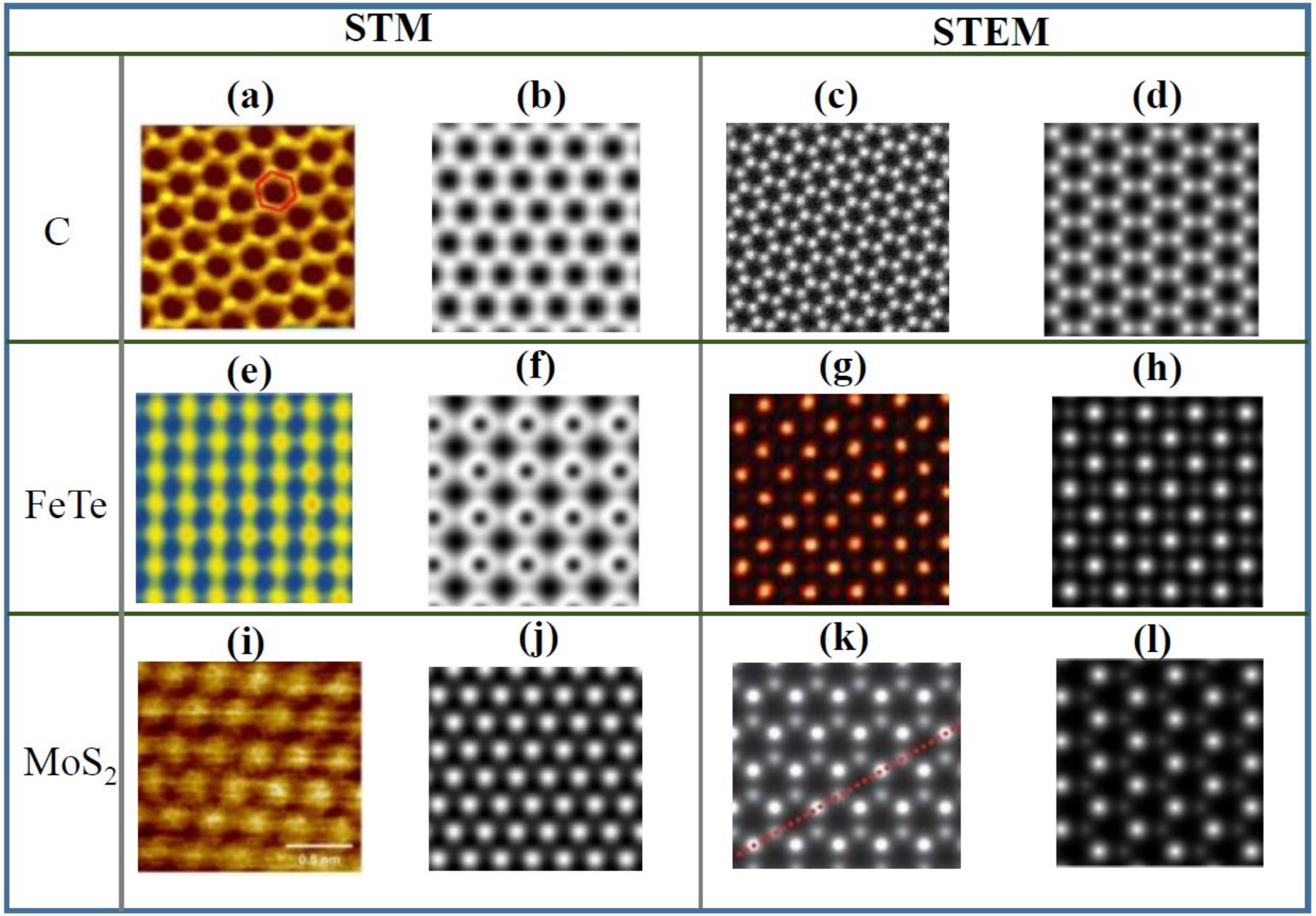
C: JVASP-667



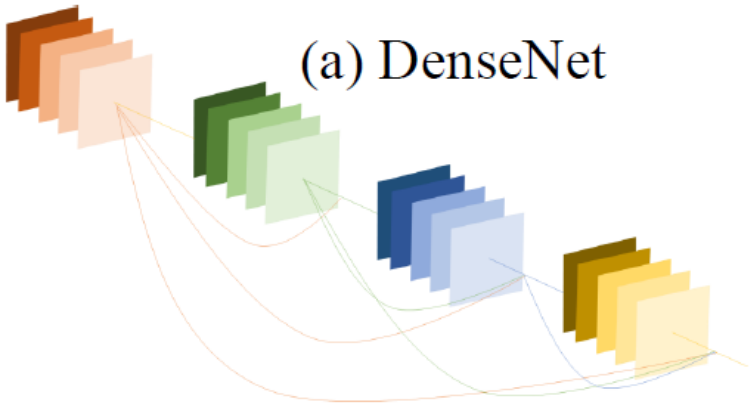
FeTe: JVASP-6667

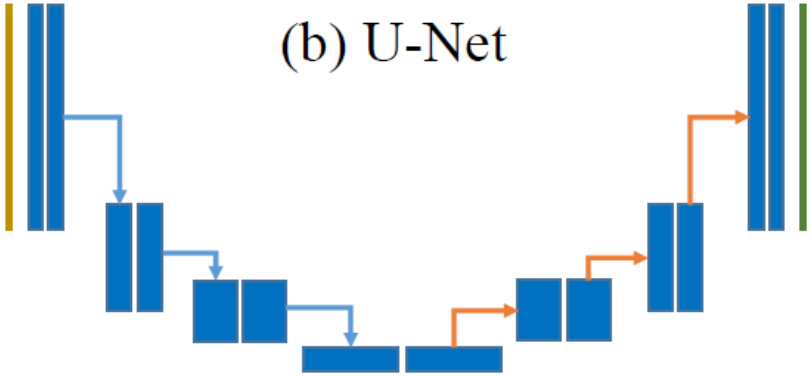
PPdSe: JVASP-6316

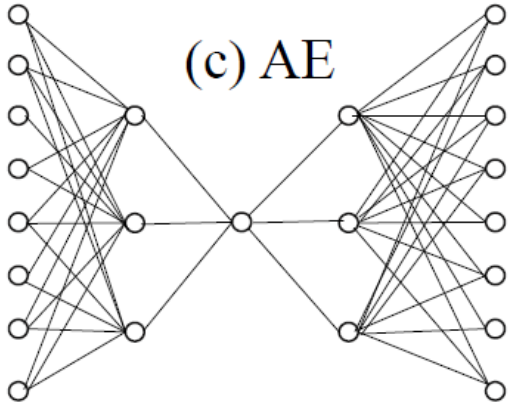
# Experimental vs computational images



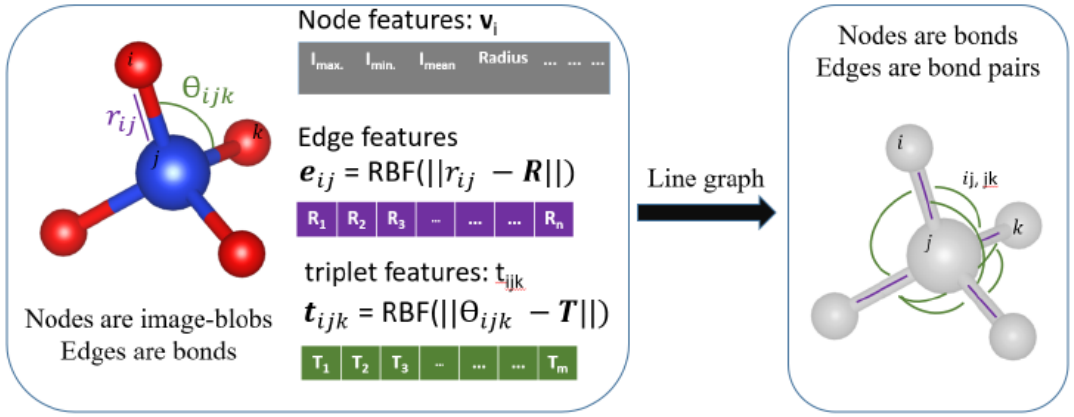
# Deep Learning architectures in AtomVision



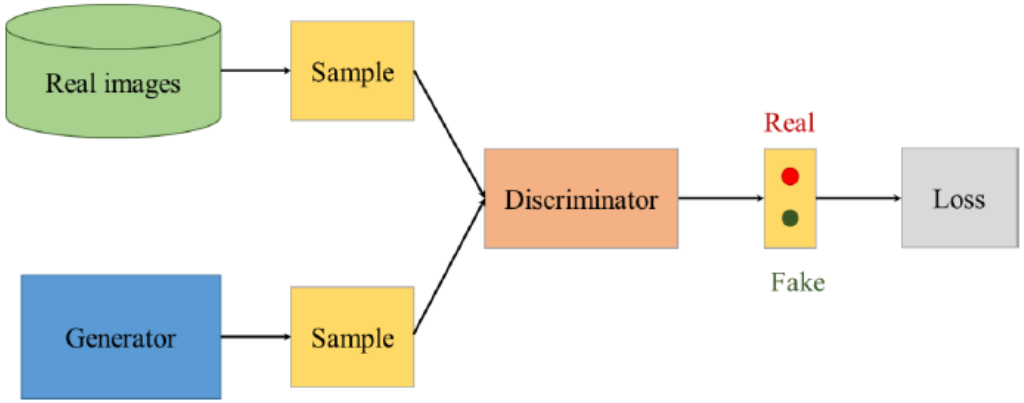




(d) ALIGNN

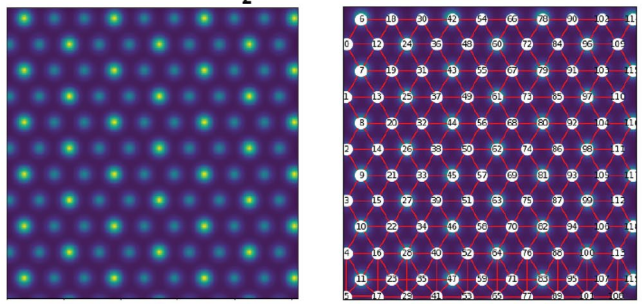



(e) SRGAN

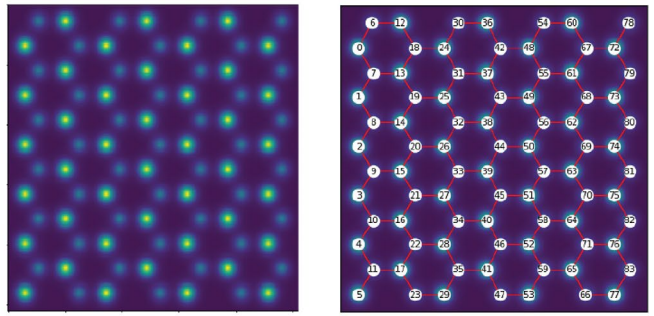


# Graph construction

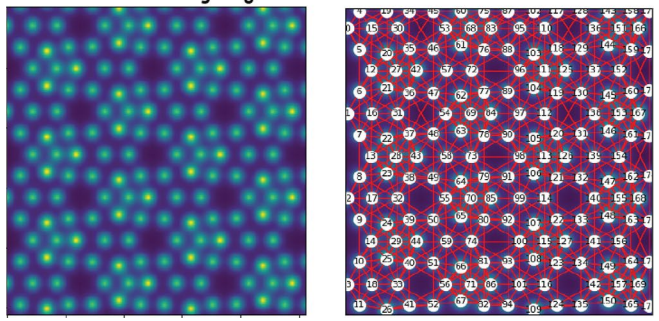
**$PbI_2$**: JVASP-76548



**GaTe**: JVASP-6838



**$Nb_3Br_8$**: JVASP-76350



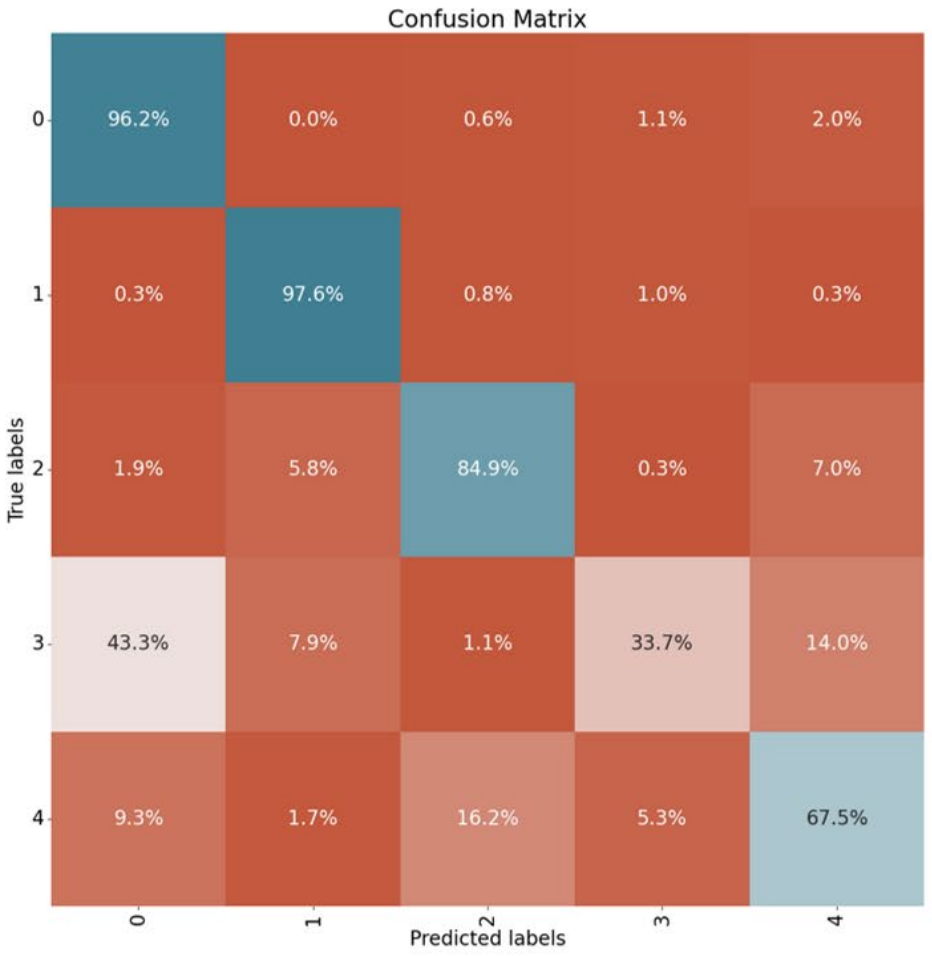
master ▾ atomvision / atomvision / scripts / train_classifier_alignn.py

Code | Blame | 388 lines (335 loc) · 10.8 KB

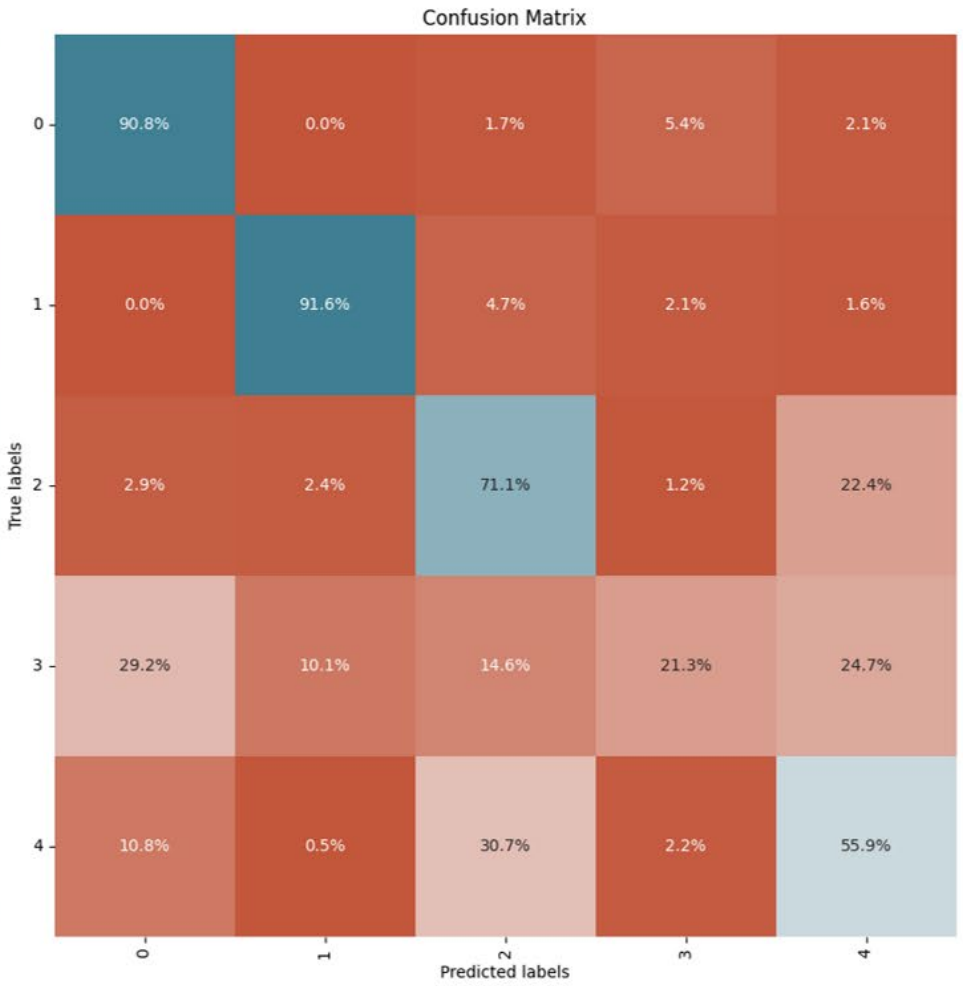
```
95  def labelled_images_to_graphs(images, labels, border_pxl=0, saveto=""):
97      Get labelled image to graph.
98
99      Args:
100         images: list of image arrays.
101
102         labels: list of corresponding class labels.
103     """
104     graphs = []
105     line_graphs = []
106     n = 0
107     for img, lbl in zip(images, labels):
108         if border_pxl != 0:
109             img = crop_image(img, border_pxl)
110         blob_list = get_blob_positions(img)
111         g, lg = blob_list_to_graph(img, blob_list)
112         graphs.append(g)
113         line_graphs.append(lg)
114         n = n + 1
115     return graphs, line_graphs
```

# Image classification (CNN & GNN)

(a) DenseNet Classifier

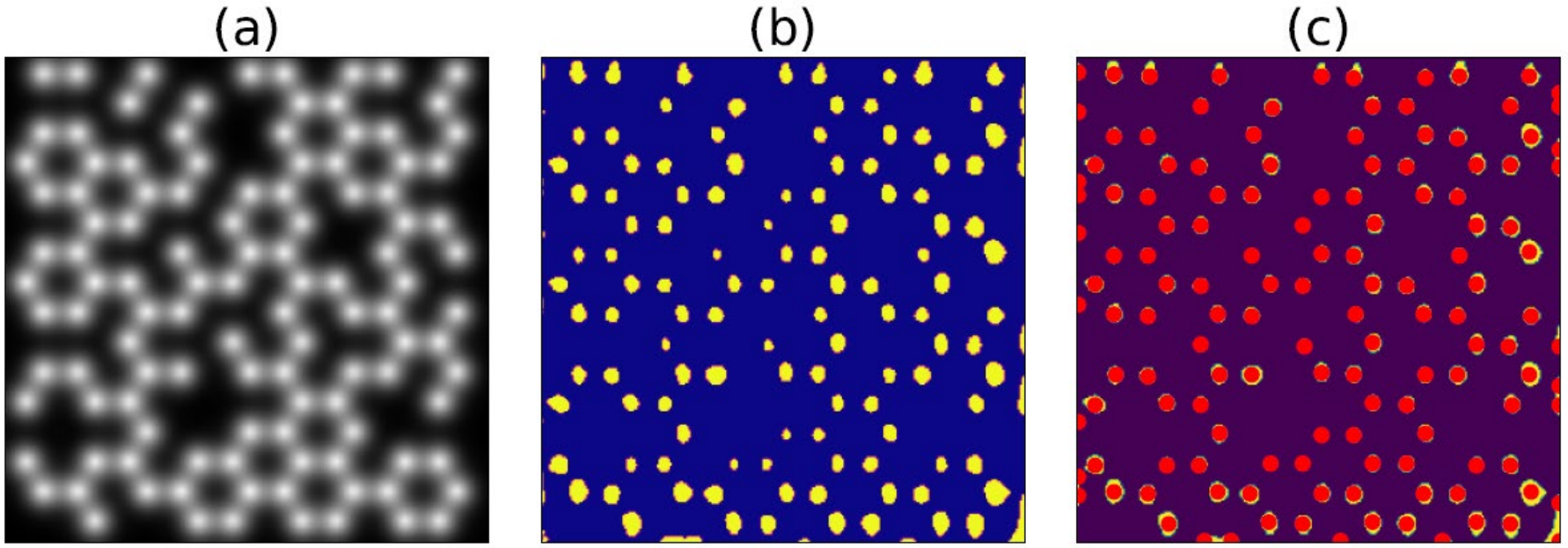



(b) ALIGNN Classifier



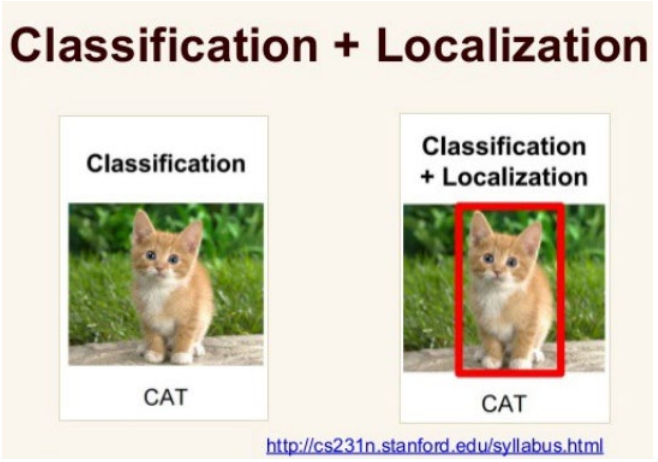

2D Bravais lattice classification (DenseNet (82%), ALIGNN(78%)):
0) hexagonal, 1) square, 2) rectangle, 3) rhombus, 4) parallelogram
Baseline accuracy 1/5 = 20 %

# Semantic segmentation



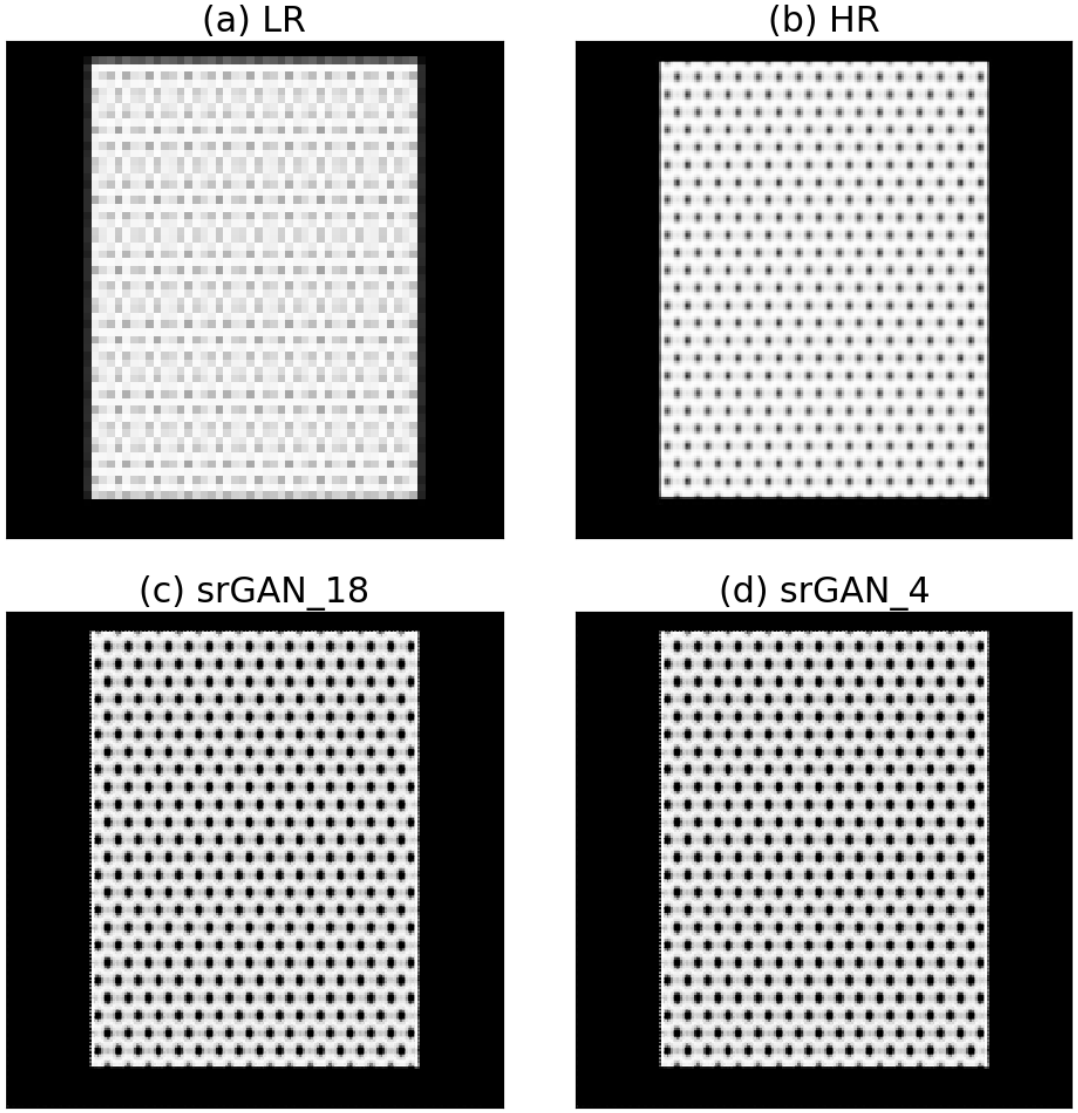

Semantic segmentation using U-Net:

- Atom vs background, pixelwise classification
- Train on computational dataset, fine-tune for experiments



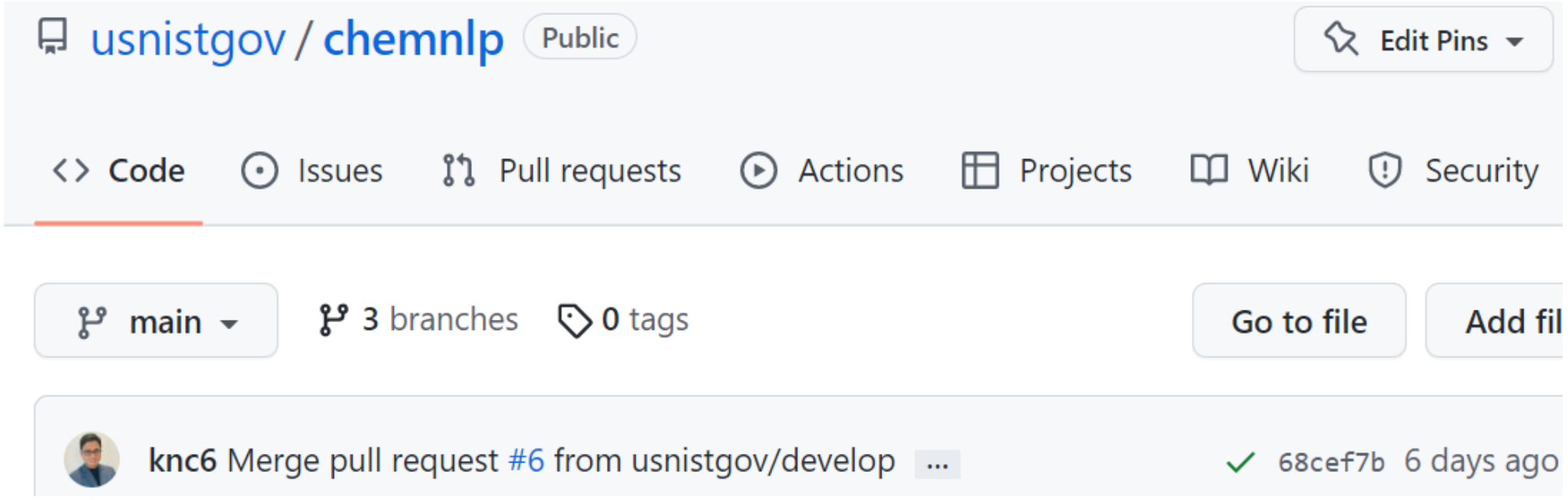
# Super-resolution

SR-GAN for enhancing image resolution with VGG19

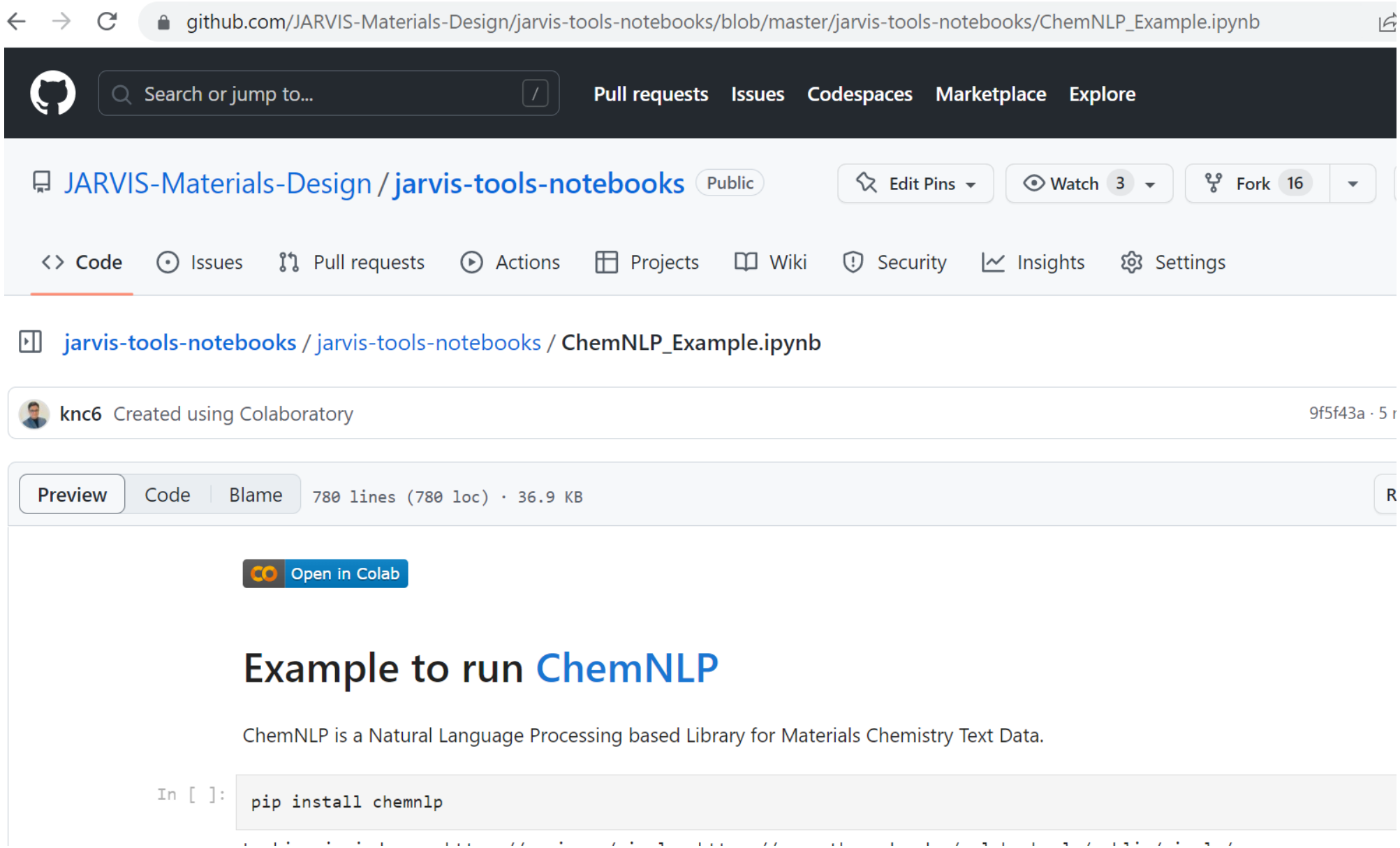


# ChemNLP

## A Natural Language Processing based Library for Materials Chemistry Text Data




# Notebook


github.com/JARVIS-Materials-Design/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/ChemNLP_Example.ipynb
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knc6 Created using Colaboratory
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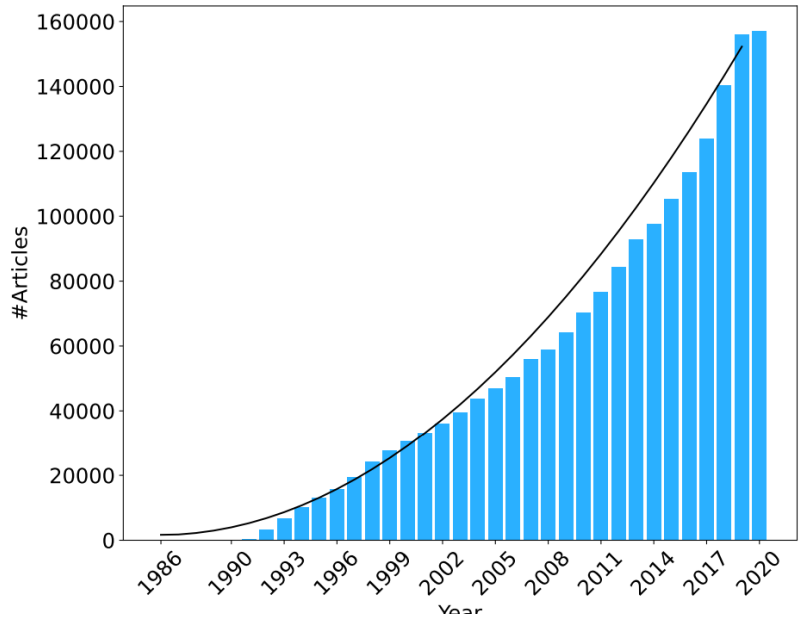
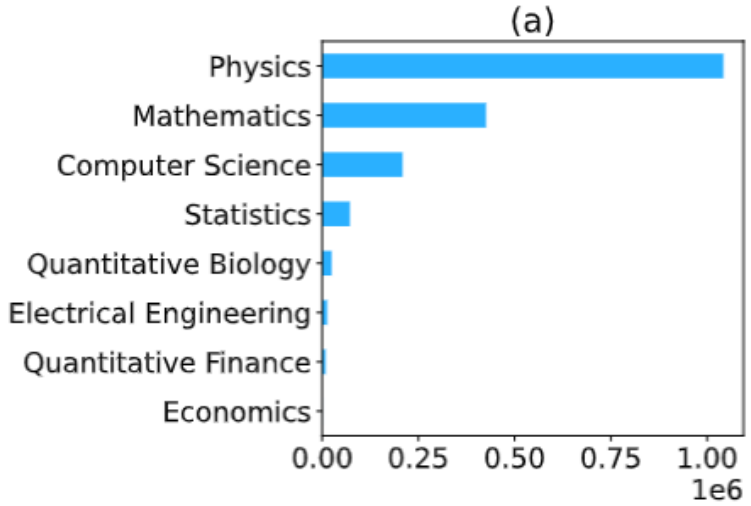
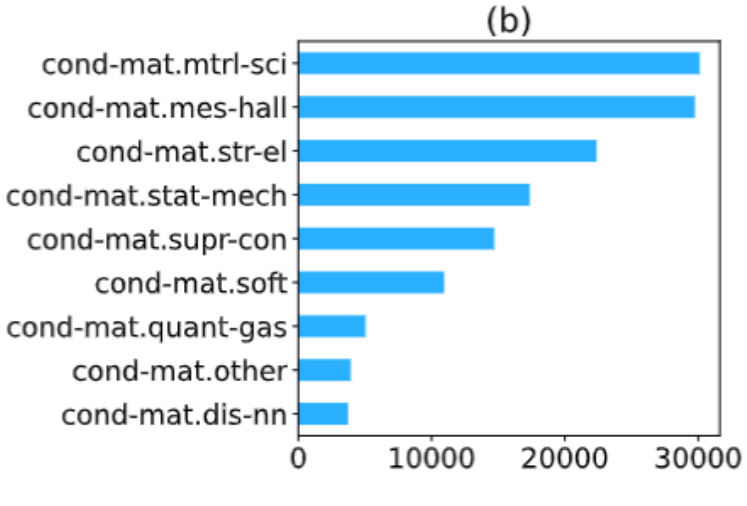
Code
Blame
780 lines (780 loc) · 36.9 KB
Open in Colab
Example to run ChemNLP
ChemNLP is a Natural Language Processing based Library for Materials Chemistry Text Data.
In [ ]:
pip install chemnlp

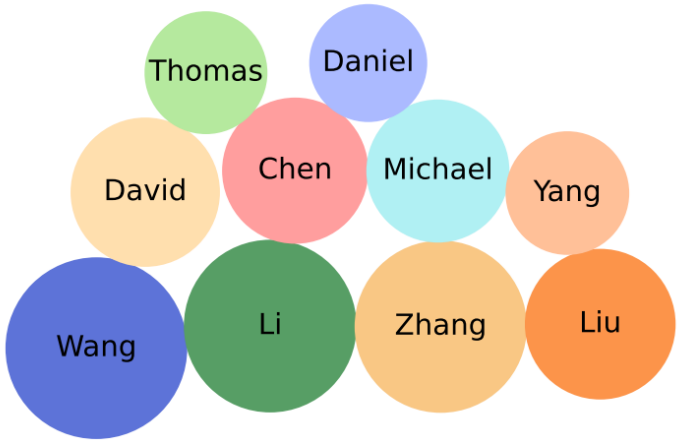
# ChemNLP

arXiv dataset 1.8 million articles




arXiv > cond-mat > arXiv:2209.08203

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**Condensed Matter > Materials Science**

*[Submitted on 17 Sep 2022]*

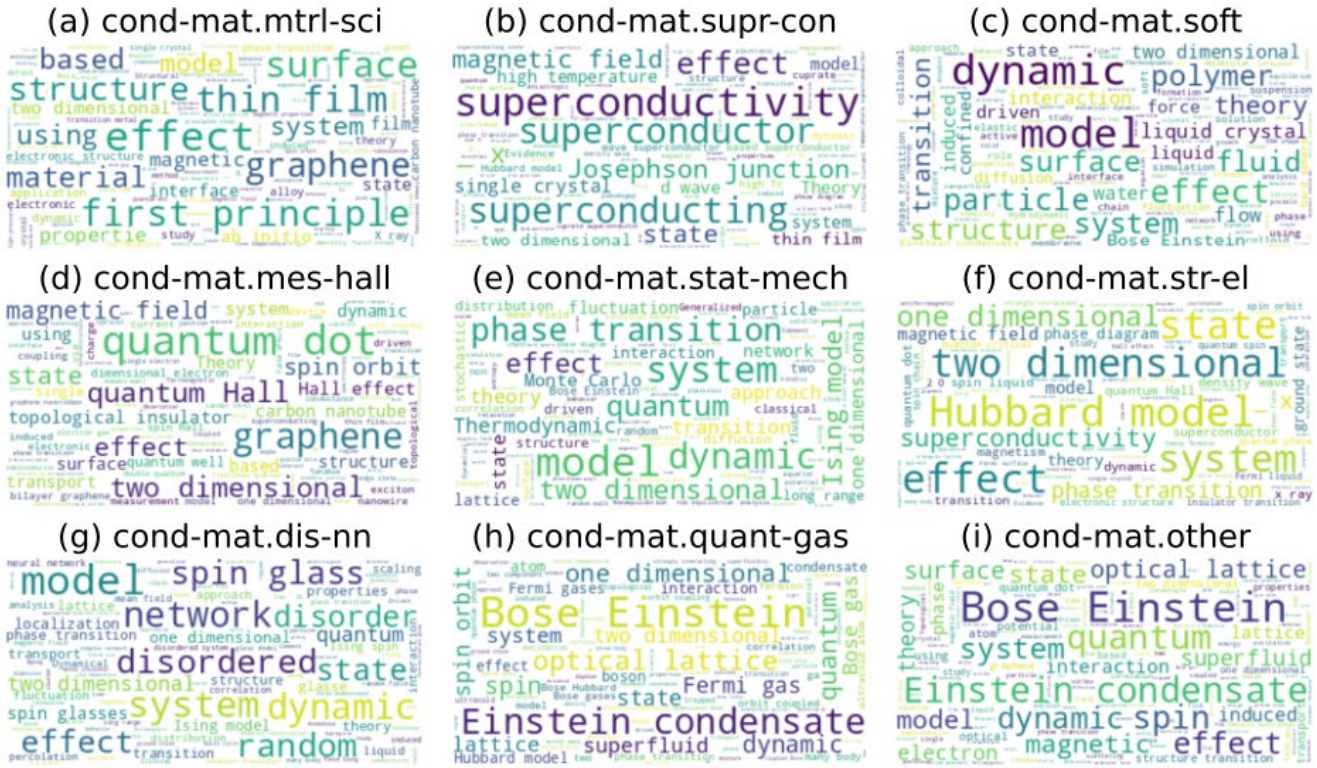
**ChemNLP: A Natural Language Processing based Library for Materials Chemistry Text Data**

Kamal Choudhary, Mathew L. Kelley

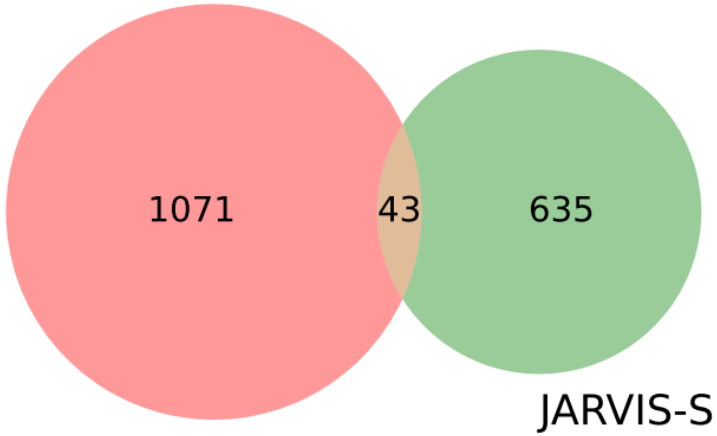
Natural language processing (NLP) has an immense potential to aid materials design processes. While there have been several advancements in this field, a complete and integrated framework with well-curated dataset and tools to apply NLP is still needed. In this work, we present the ChemNLP library and an accompanying web-app that can be used to analyze important materials chemistry information. We use the publicly available arXiv dataset that has been collected over 34 years and contains ~1.8 million articles. First, we analyze the article publication trend, categorizations, and common phrases in the arXiv dataset. Then, we develop a user-friendly, interactive web-app to retrieve articles for a given chemical compound. Furthermore, we demonstrate the effectiveness of the proposed framework to accelerate the identification of superconducting materials. We determine the overlap between density functional theory and text-based databases for superconductors. Finally, we perform machine learning based clustering and classification tasks to quickly categorize scholarly articles given article title information with accuracy up to 81.2 %. ChemNLP is available at the websites: this https URL and this https URL.

arXiv:2209.08203

# ChemNLP



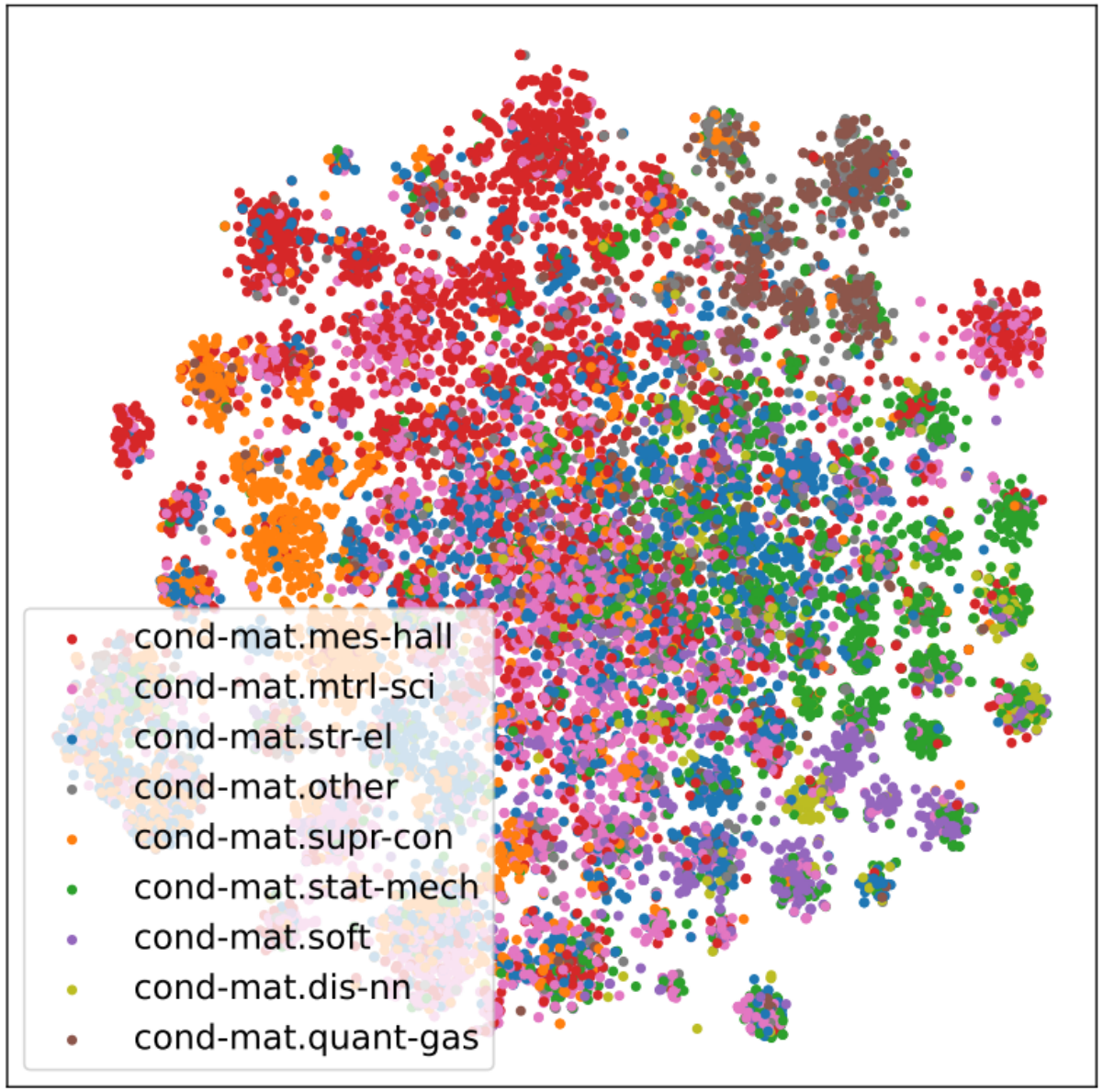

Word-cloud




Venn diagram for chemical formula available in arXiv cond-mat.supr-con and JARVIS-SuperconDB

arXiv:2209.08203

# ChemNLP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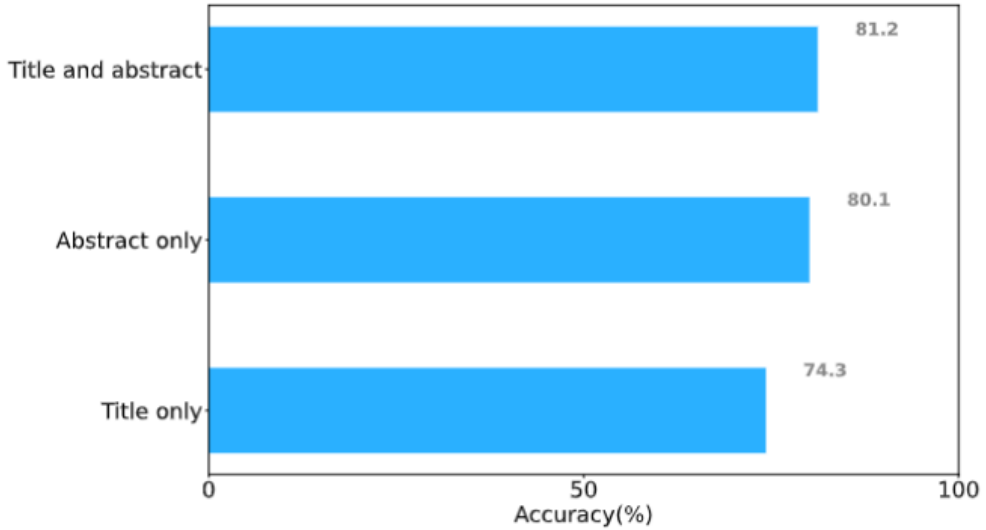
Title and abstract
81.2
Abstract only
80.1
Title only
74.3
0
50
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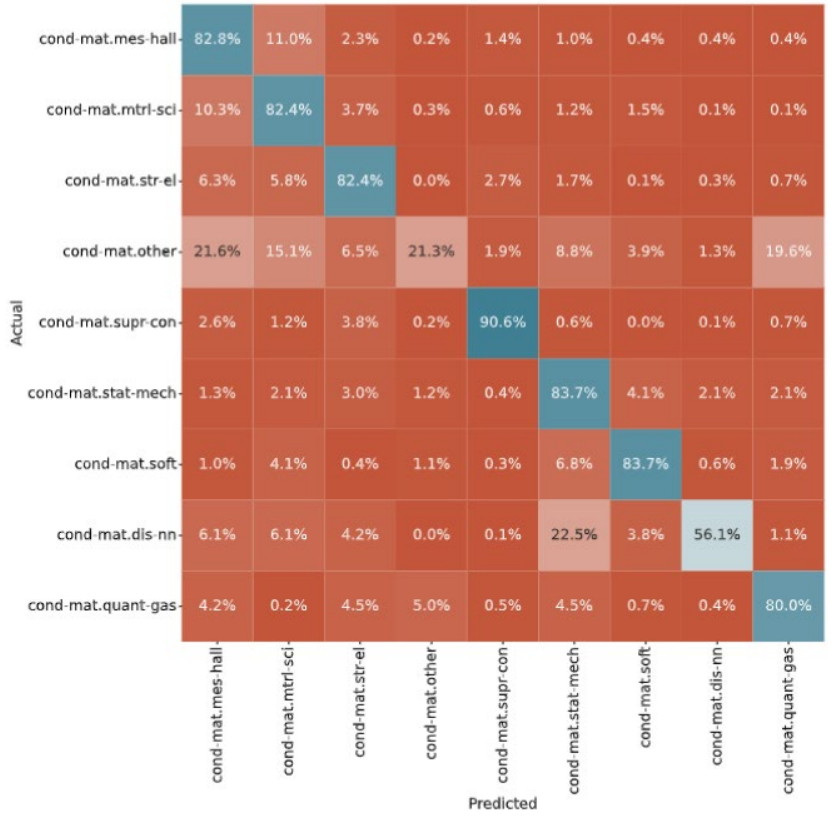
Accuracy(%)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cond-mat.quant-gas 4.2% 0.2% 4.5% 5.0% 0.5% 4.5% 0.7% 0.4% 80.0%
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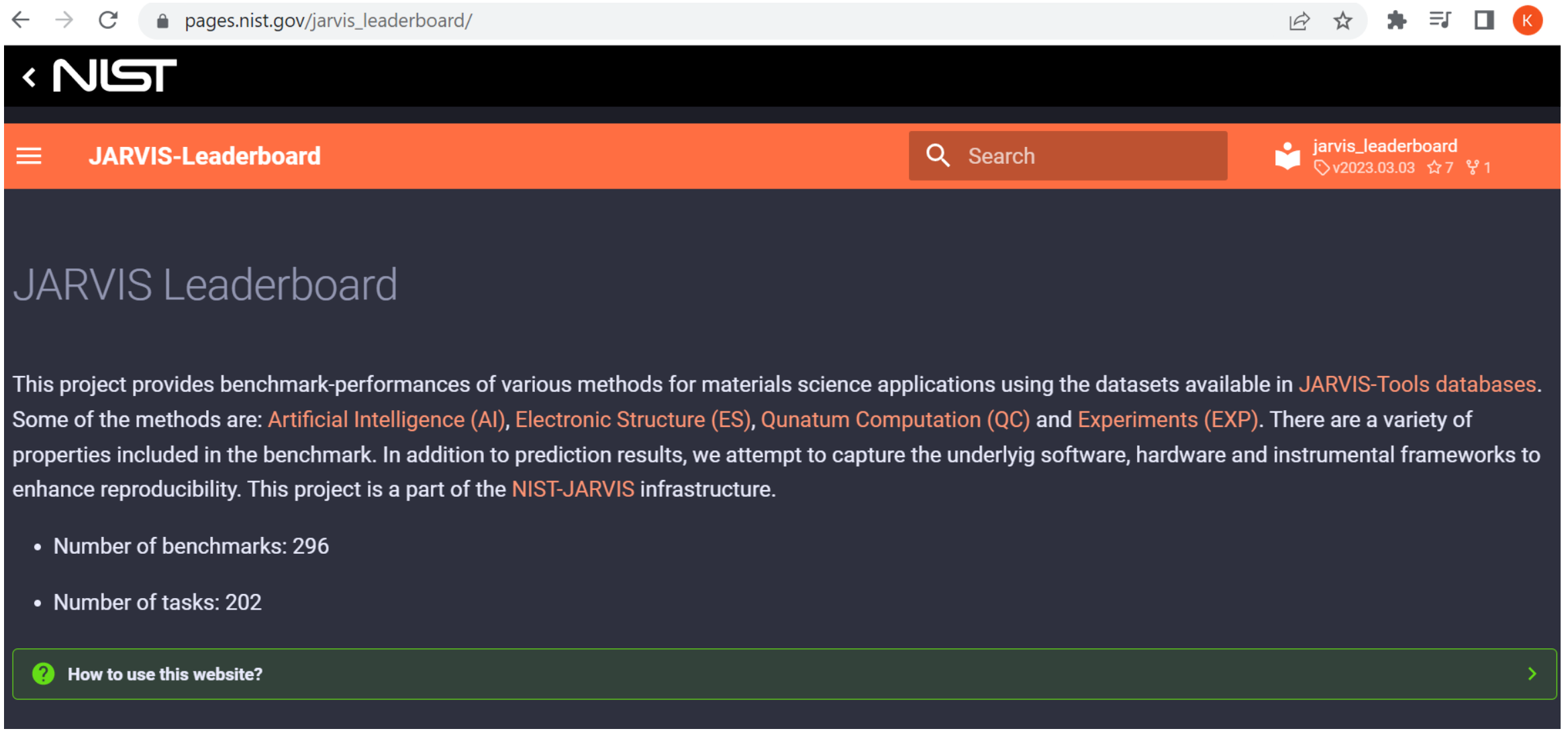
Predicted

# JARVIS-Leaderboard



# Summary & future works

- Deep-learning for various data-types
- Many state-of-the-art models achieved with GNNs
- Notebooks and GitHub repos; contributions welcome!
- GNN and other methods for benchmarking

Slides:https://www.slideshare.net/KAMALCHOUDHARY4

Email: kamal.choudhary@nist.gov

JARVIS

LinkedIn

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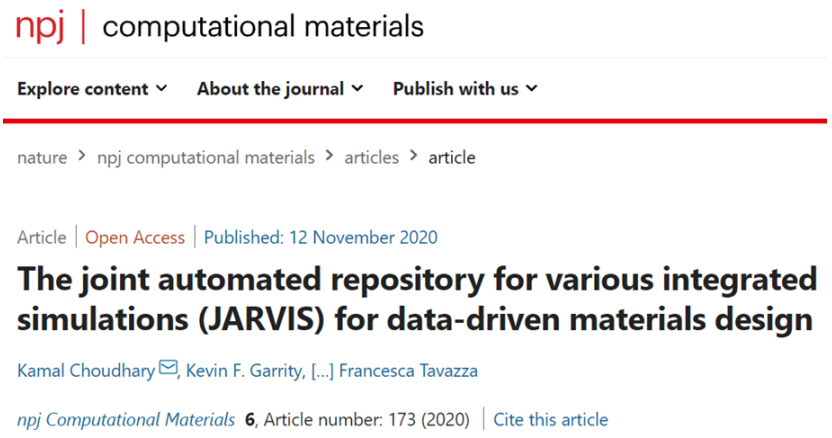


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