Materials Informatics: Fingerprints, Graph Neural Networks, and Transformers Based Models for Materials Design

Estd. 1901

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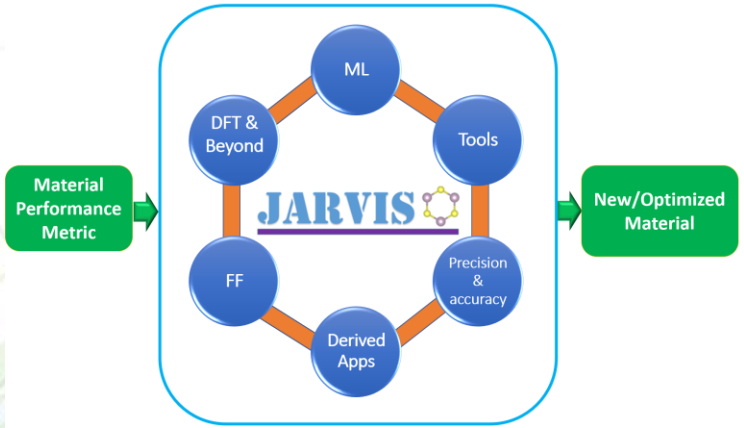
Jan 20-25, 2025



https://jarvis.nist.gov

Joi[illegible] Integ[illegible]ations

NIST NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Outline

Day 1 Materials Science Basics

Modeling Materials & its applications

Programming

Quantum mechanics

Classical mechanics

MSE experiments

Day 2 AI/ML Basics

Types of ML & Models

Workflow

Databases

Classical ML (CFID, MatMiner,…)

Day 3 Deep Learning Models

CNN (AtomVision)

GNN (ALIGNN, ALIGNN-FF)

GPT (AtomGPT, DiffractGPT)

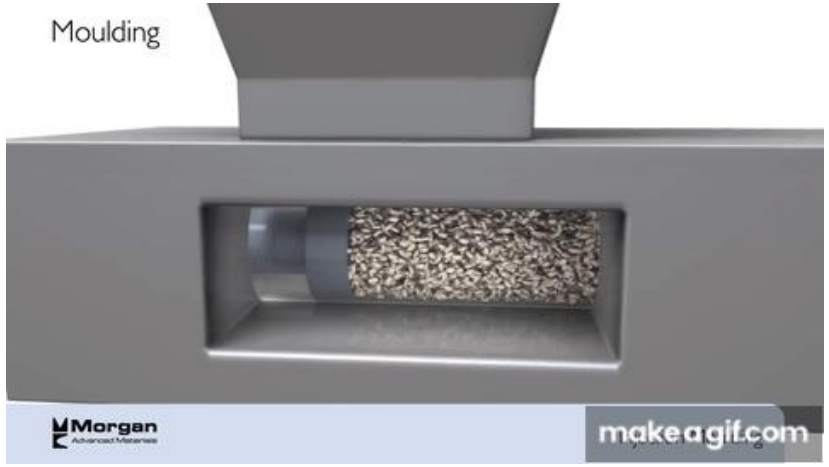
Benchmarking and reproducibility (JARVIS-Leaderboard)

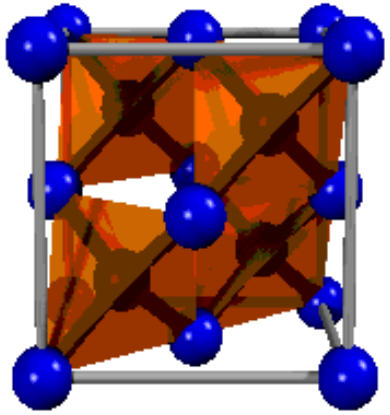
Day 1 Schedule

- Fundamentals of Materials Science, Modeling, Programming
- Quantum Mechanical Calculations
- Classical Calculations

Materials Science Basics: PSPP

- **Material Definition**: A material is a substance or mixture of substances that forms an object. It can be pure or impure and include both living or non-living matter.
- **PSPP Relationship**: Fundamental concept in materials science linking processing, structure, properties, and performance.
- **Processing**: Methods and conditions under which a material is produced.
  - **Example**: Heat treatments like annealing and quenching alter mechanical properties such as toughness and ductility.
- **Structure**: Arrangement of atoms and molecules in a material, from nanostructures to macrostructures.
  - **Example**: Grain size in metals controlled through rolling or annealing, affecting strength via the Hall-Petch effect.

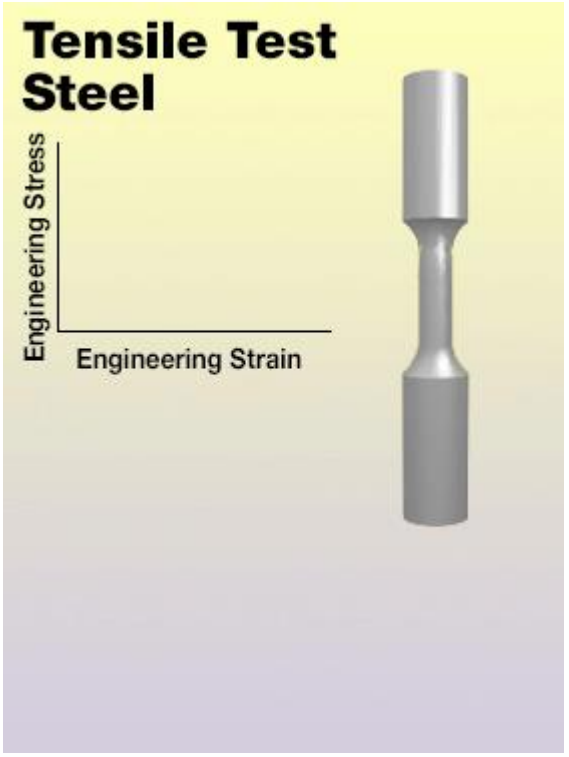




Diamond crystal structure - Wikimedia

Materials Science Basics: PSPP

- **Properties**: Measurable material behaviors including mechanical, electrical, and thermal properties.
  - **Example**: strength, ductility, and elasticity of steel
- **Performance**: How a material behaves under real-world conditions.
  - **Example**: Tensile test results for engineers to predict the steel's performance under load



https://www.mtu.edu/materials/k12/experiments/tensile/

Materials Science

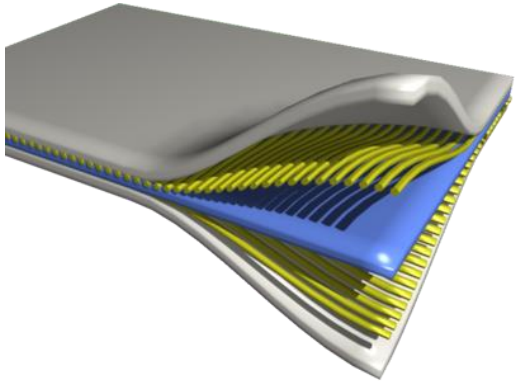
Material Classes

1. **Metals**
   - aluminum
   - copper
   - steel (iron alloy)
   - nickel
   - titanium

2. **Ceramics**
   - clay
   - silica glass
   - alumina
   - quartz

3. **Polymers**
   - polyvinyl chloride (PVC)
   - Teflon
   - various plastics
   - glue (adhesives)
   - Kevlar

4. **Composites**
   - wood
   - carbon fiber resins
   - concrete

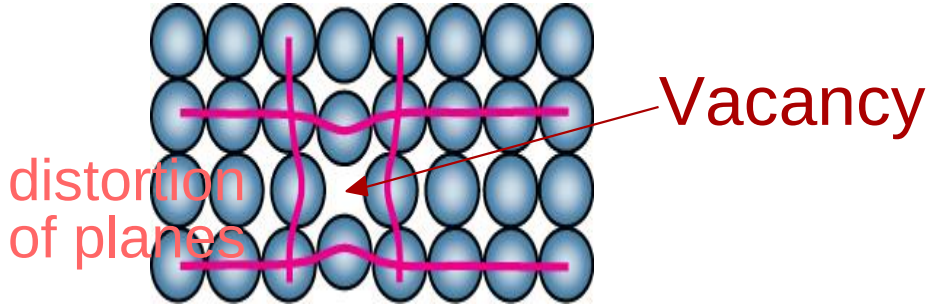


- Solids/Liquids/Gases
- Crystalline/Amorphous

Perfect vs Defects Materials

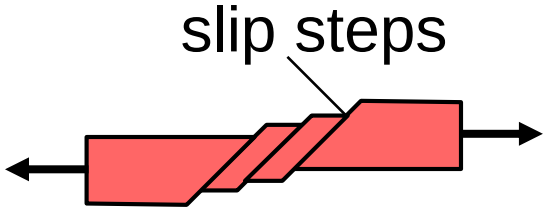
- Vacancy atoms
- Interstitial atoms
- Substitutional atoms

Point defects



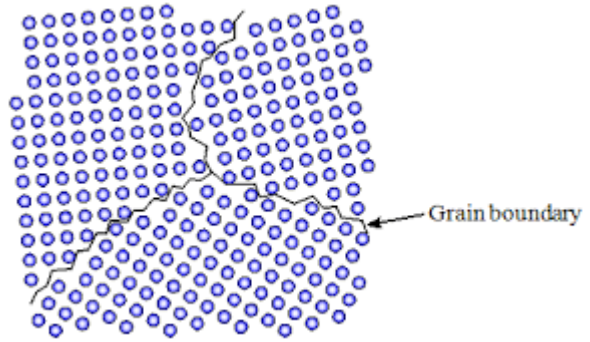
- Dislocations

Line defects



- Surfaces, Grain Boundaries

Area defects

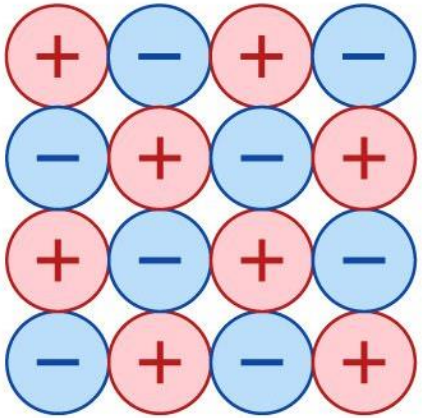


Crystal Systems

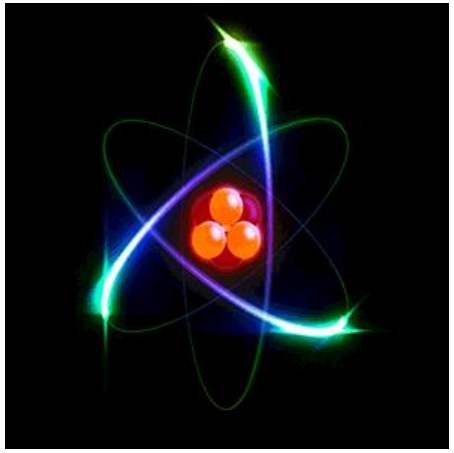
Crystal System	Bravais Lattice Types	Unit Cell Characteristics	Examples
Cubic	Simple (P), Body-Centered (I), Face-Centered (F)	$a = b = c, \alpha = \beta = \gamma = 90^\circ$	NaCl, CsCl, Diamond
Tetragonal	Simple (P), Body-Centered (I)	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$	SnO_2 (Rutile), In, TiO_2
Orthorhombic	Simple (P), Body-Centered (I), Face-Centered (F), Base-Centered (C)	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$	Olivine, $BaSO_4$, KNO_3
Hexagonal	Simple (P)	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	Graphite, ZnO, Mg
Trigonal	Simple (P)	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	Calcite, Quartz (α-quartz)
Monoclinic	Simple (P), Base-Centered (C)	$a \neq b \neq c, \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$	Gypsum, Mica, Clinopyroxene
Triclinic	Simple (P)	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$	Kyanite, $CuSO_4 \cdot 5H_2O$, Turquoise

Chemical Bonding

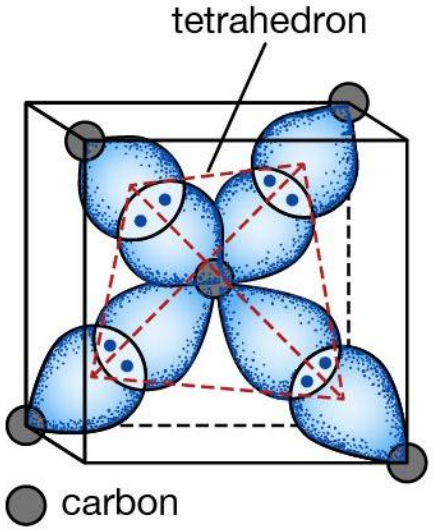
ionic bond



An idealized ionic (or electrovalent) bonding of oppositely charged ions.

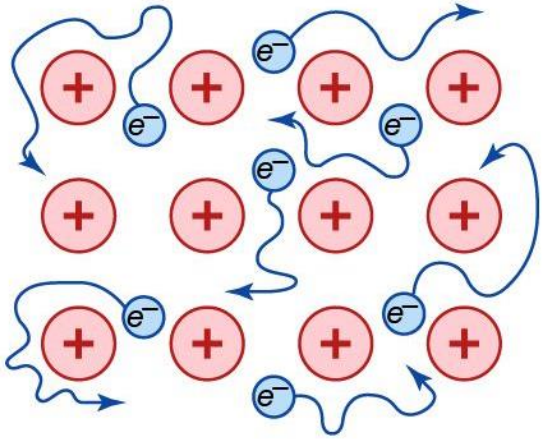


covalent bond



Covalent bonds involve electron sharing, such as between these carbon atoms when they form a diamond.

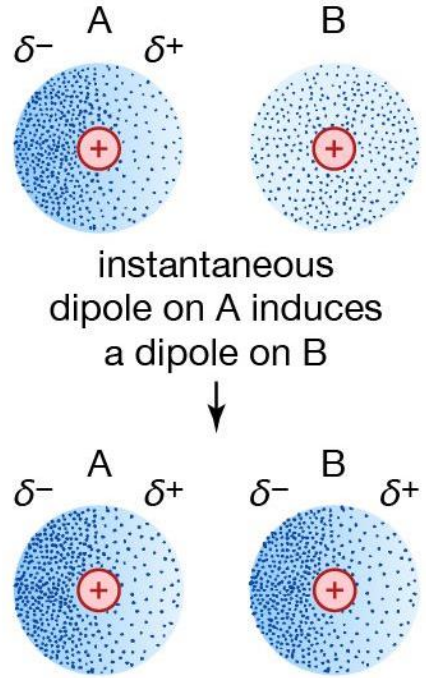
metallic bond



metallic structure, showing possible electron (e^-) paths around the nuclei of metal atoms (represented as spheres with a positive charge)

Metallic bonding can be thought of as a cloud of positively charged ions immersed in a cloud of valence electrons.

van der Waals bond



Neutral molecules may be held together by a weak electric force known as the van der Waals bond.

Chemical Bonding

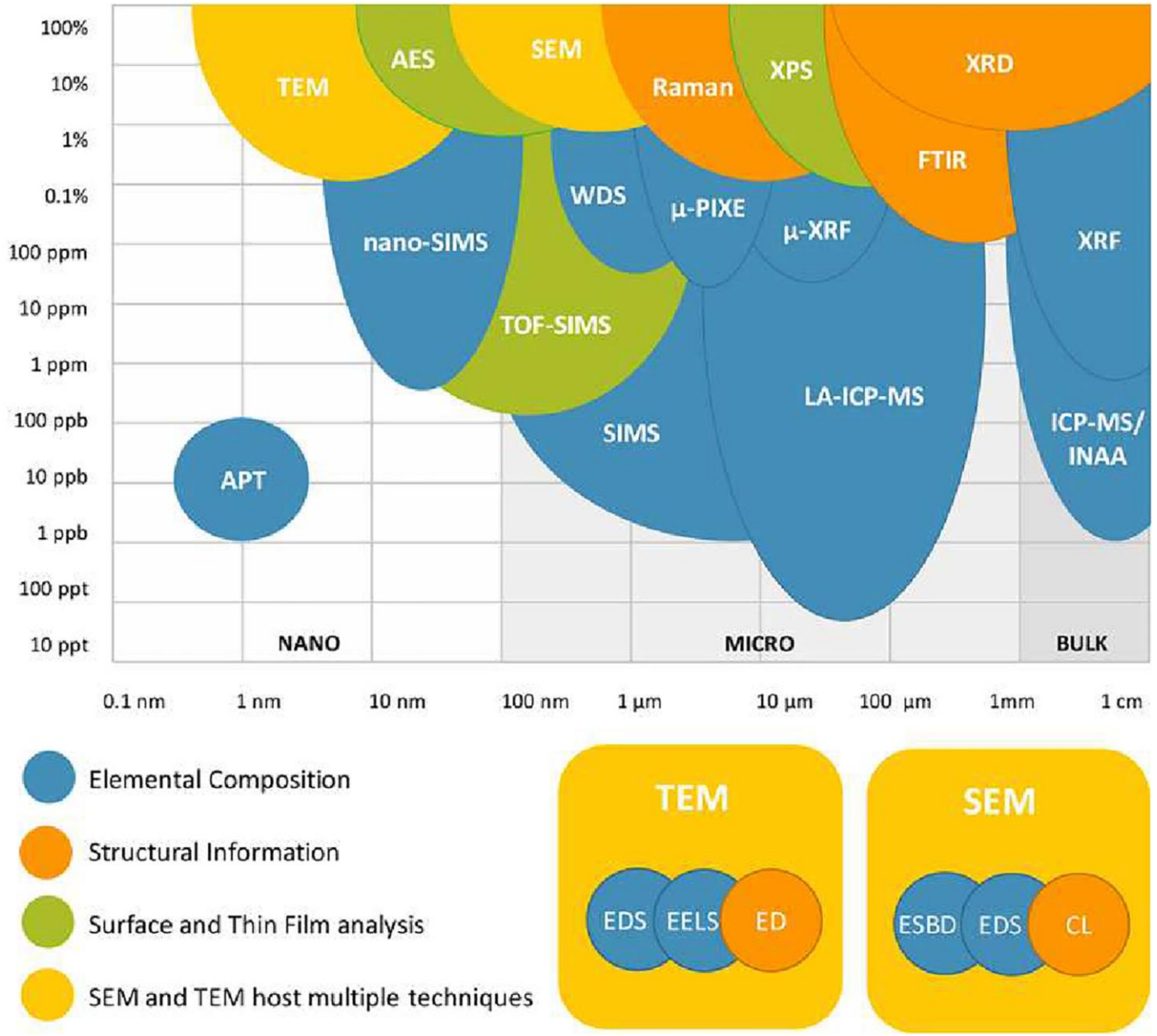
- **Metals: Metallic Bonding**
  - Delocalized electrons create a "sea" around positive ions.
  - **Properties**: Conductivity, malleability, ductility, luster.

- **Ceramics: Ionic and Covalent Bonding**
  - **Ionic**: Electron transfer between metal and non-metal, forming charged ions.
  - **Covalent**: Electron sharing, generally between non-metals, leading to directional and strong bonds.
  - **Properties**: Hardness, brittleness, high melting point, chemical stability.

- **Polymers: Covalent Bonding**
  - Long chains of molecules connected by strong covalent bonds.
  - **Properties**: Elasticity, plasticity, tensile strength, chemical resistance.

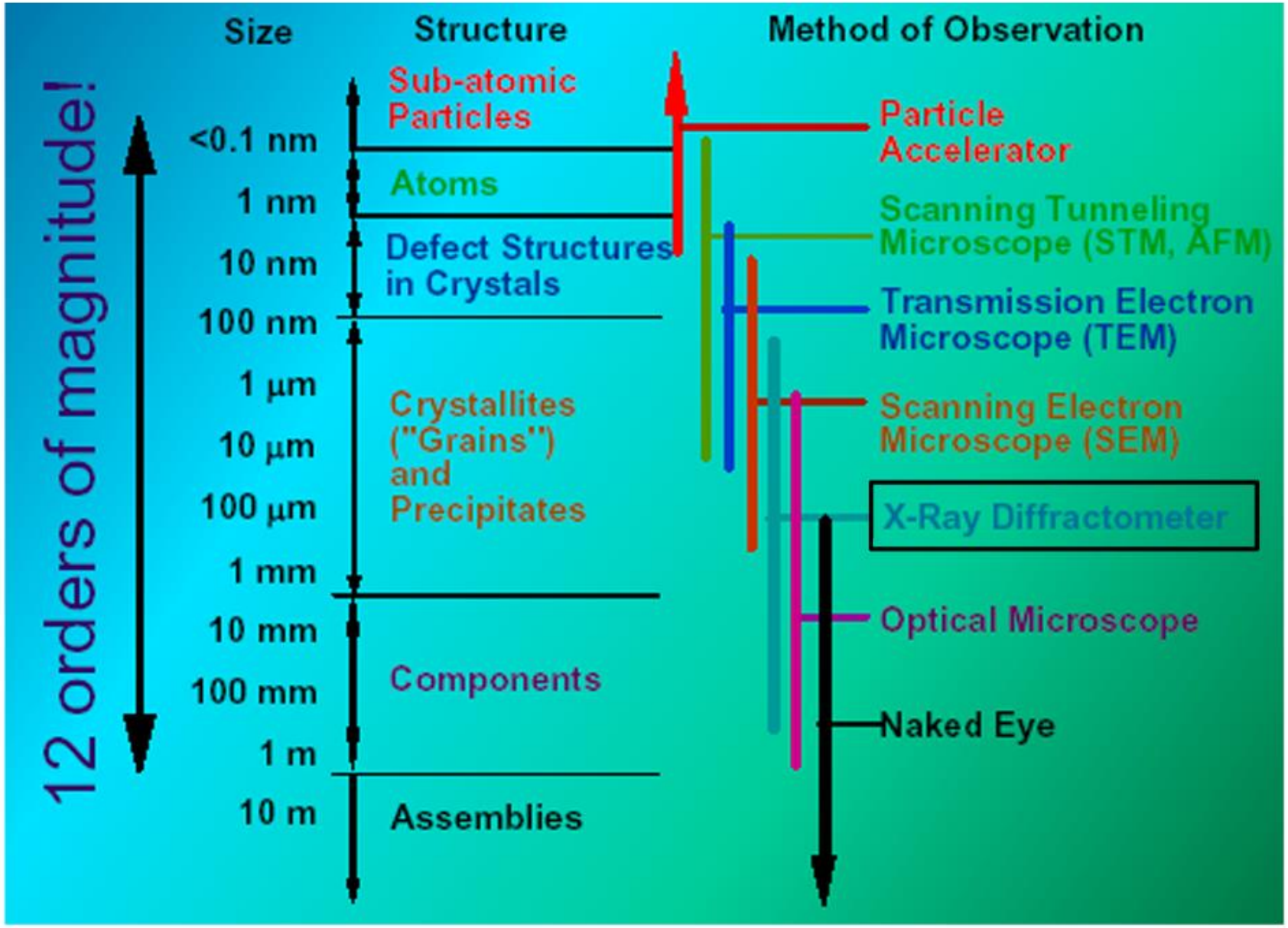
- **Composites: Varied Bonding**
  - Combinations of different materials, each retaining its own bonding characteristics.
  - **Properties**: Enhanced mechanical properties, tailored functionalities, improved durability.

Materials Characterization



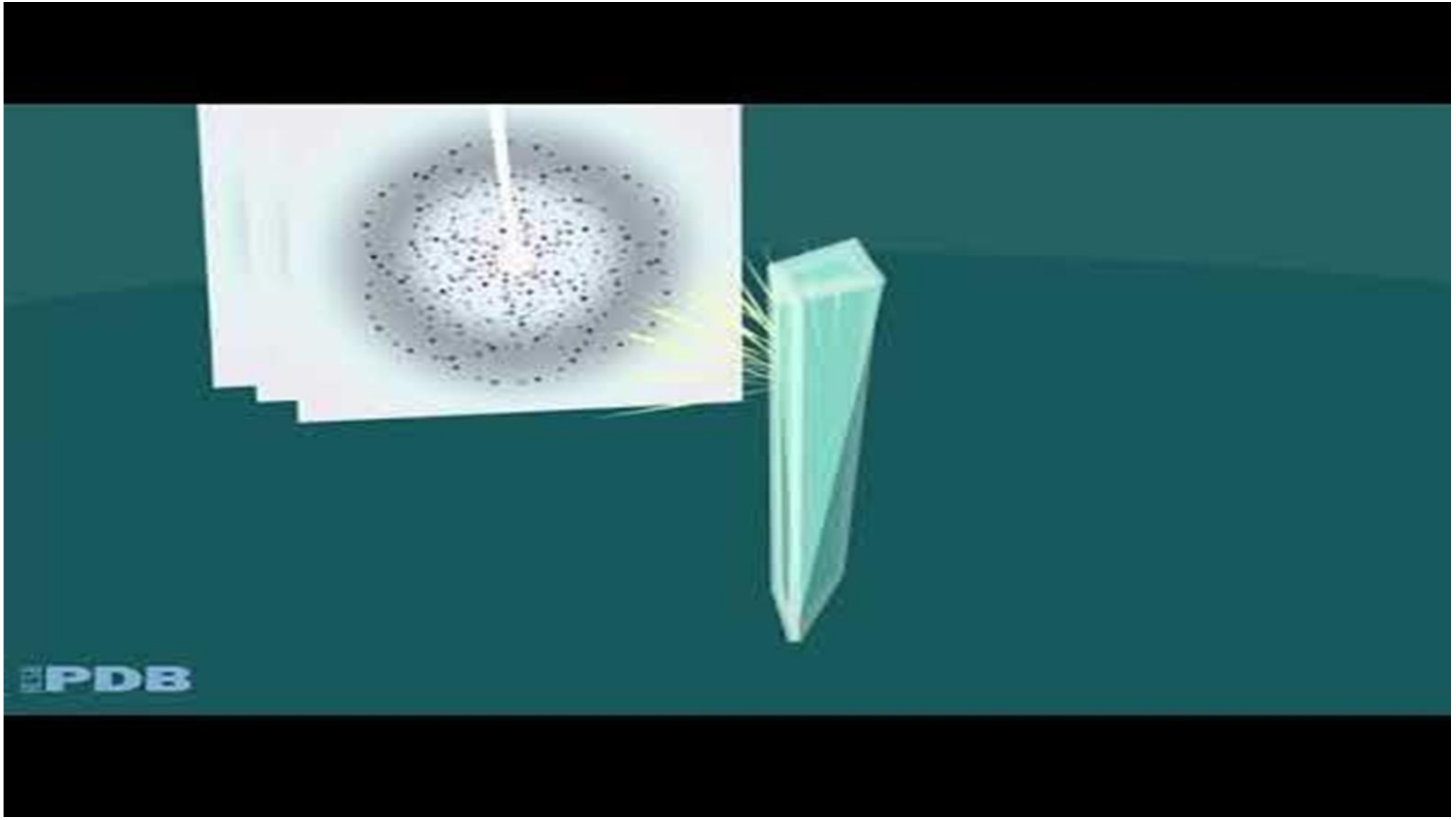
https://onlinelibrary.wiley.com/doi/10.1002/cjce.25218

Materials Characterization



https://www.iitk.ac.in/che/PG_research_lab/pdf/resources/XRD-reading-material.pdf

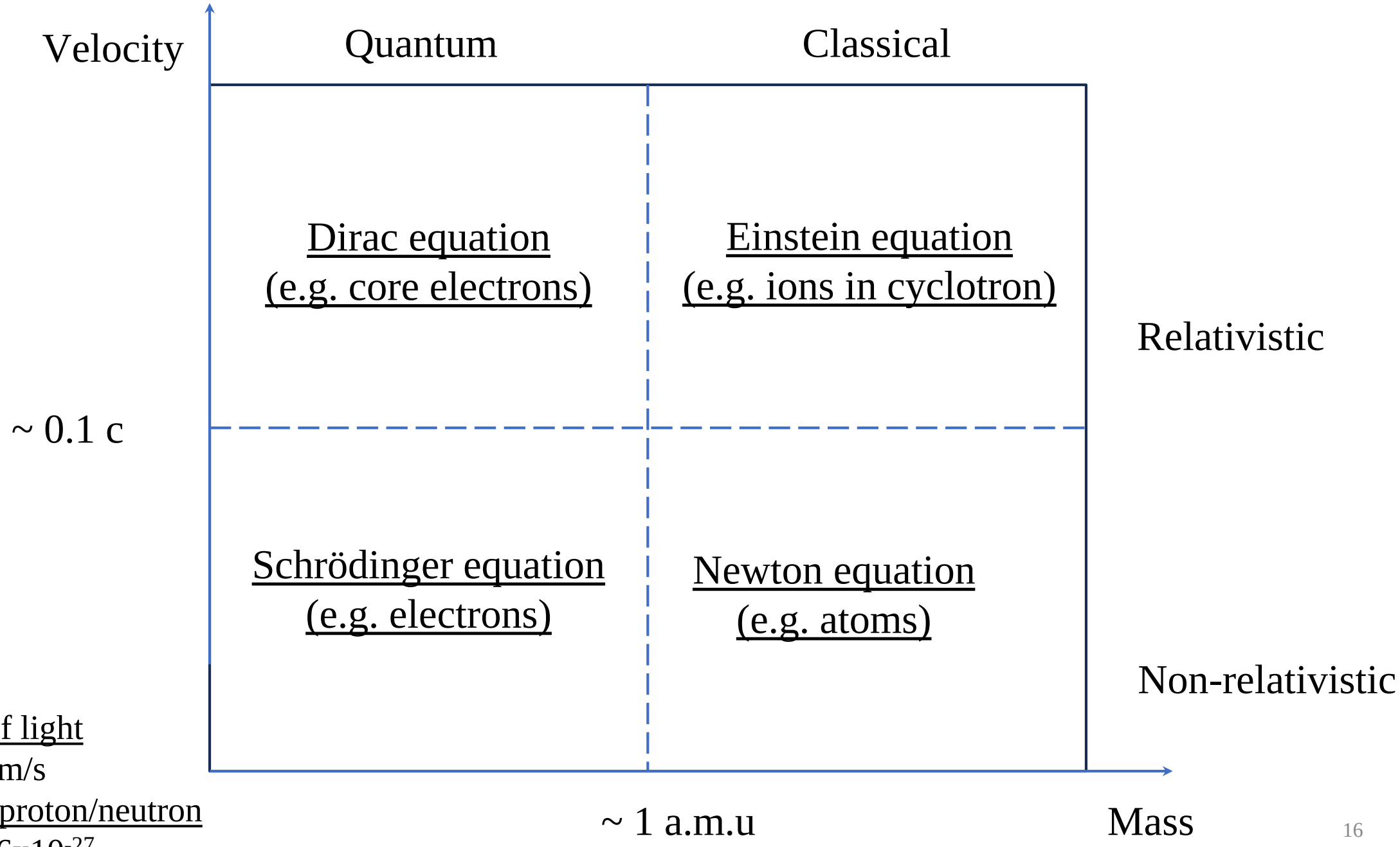
X-ray Crystallography



https://www.youtube.com/watch?v=RUok4O9oovQ

What is a Model?

- **Definition of a Model**: A simplified representation of reality to analyze, understand, or predict real-world phenomena.
- **Purpose of Models**:
  - Simulate complex systems or phenomena.
  - Illustrate or reason about specific aspects of the real world.
  - Aid in decision-making in research, development, policy-making, and education.
- **Types of Models**:
  - **Physical Models**: Tangible, scaled-down versions of objects (e.g., globes, architectural models).
  - **Mathematical Models**: Use mathematical expressions to describe system variables (common in physics, economics, engineering).
  - **Statistical Models**: Apply statistical methods to infer and predict data patterns (e.g., linear regression, machine learning algorithms).
  - **Conceptual Models**: Diagrams or flowcharts simplifying complex ideas (used in biology, management).
  - **Computational Models**: Algorithms and simulations for studying complex system behavior (e.g., climate models, atomic simulations).



Velocity of light
$c = 3x10^{8}$ m/s

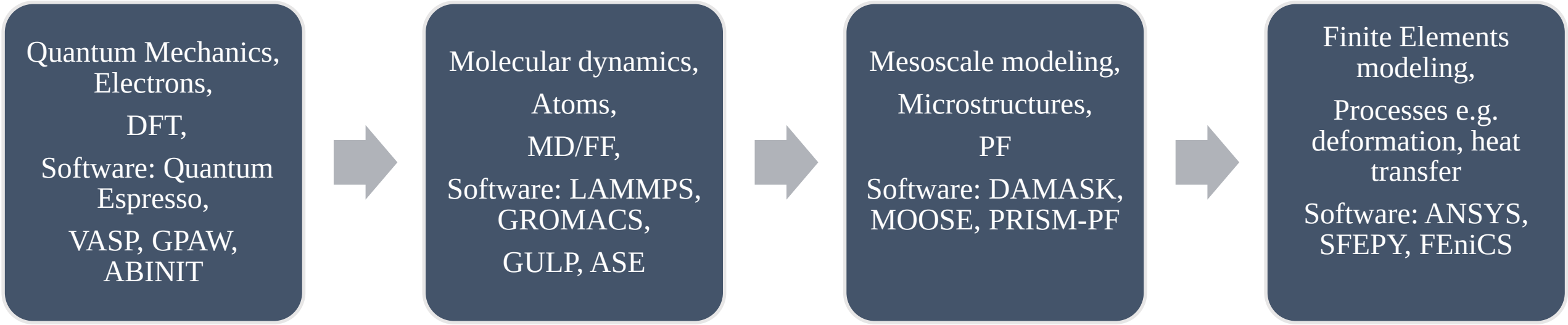
Mass of a proton/neutron
amu = $1.66x10^{-27}$

Multiscale Modeling for Mechanical Systems

Multiscale modeling is a computational approach that

- **integrates** models at different **spatial and temporal** scales to simulate complex systems.

- crucial in mechanical systems, where phenomena at one scale can **significantly influence** other scales.



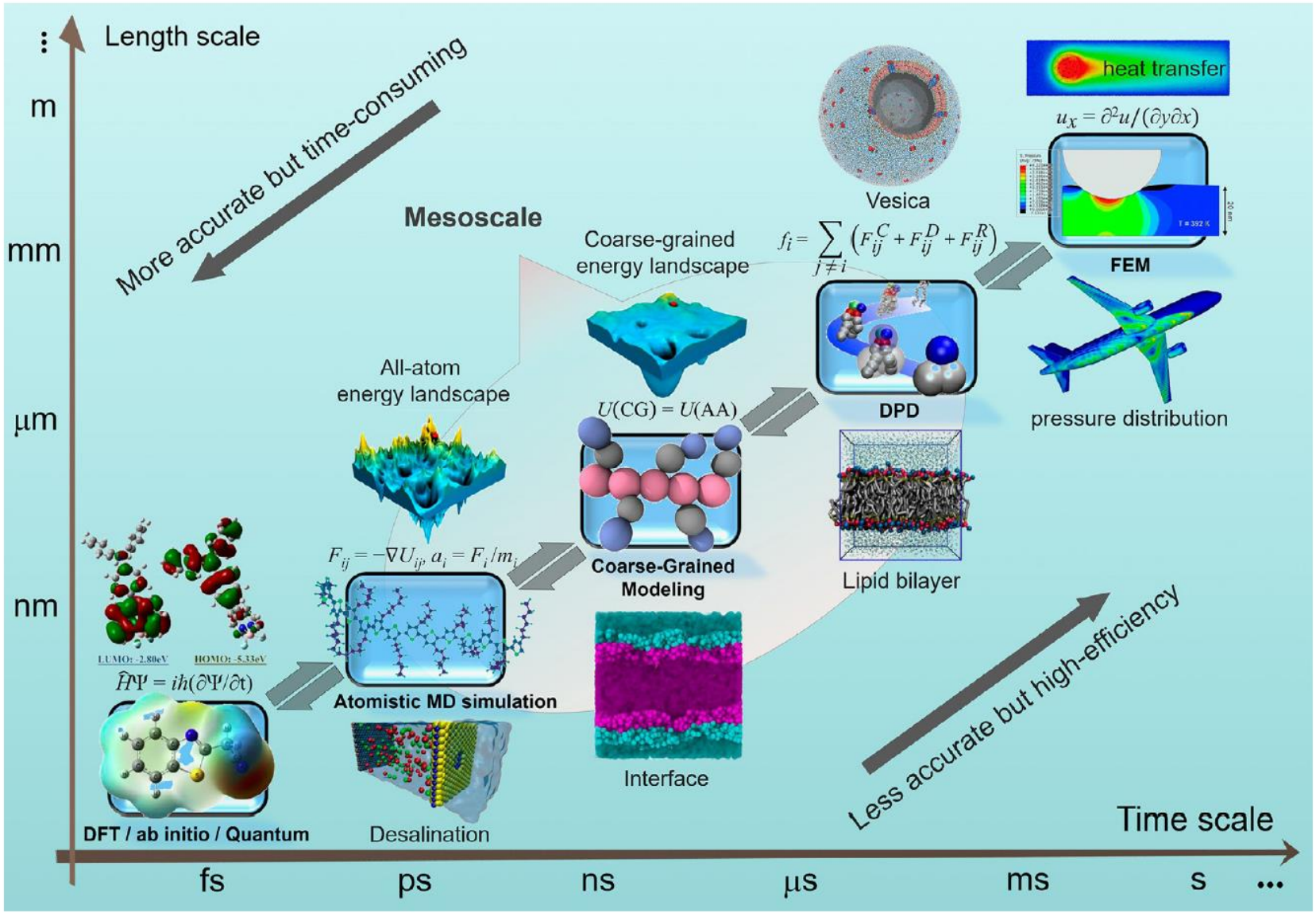
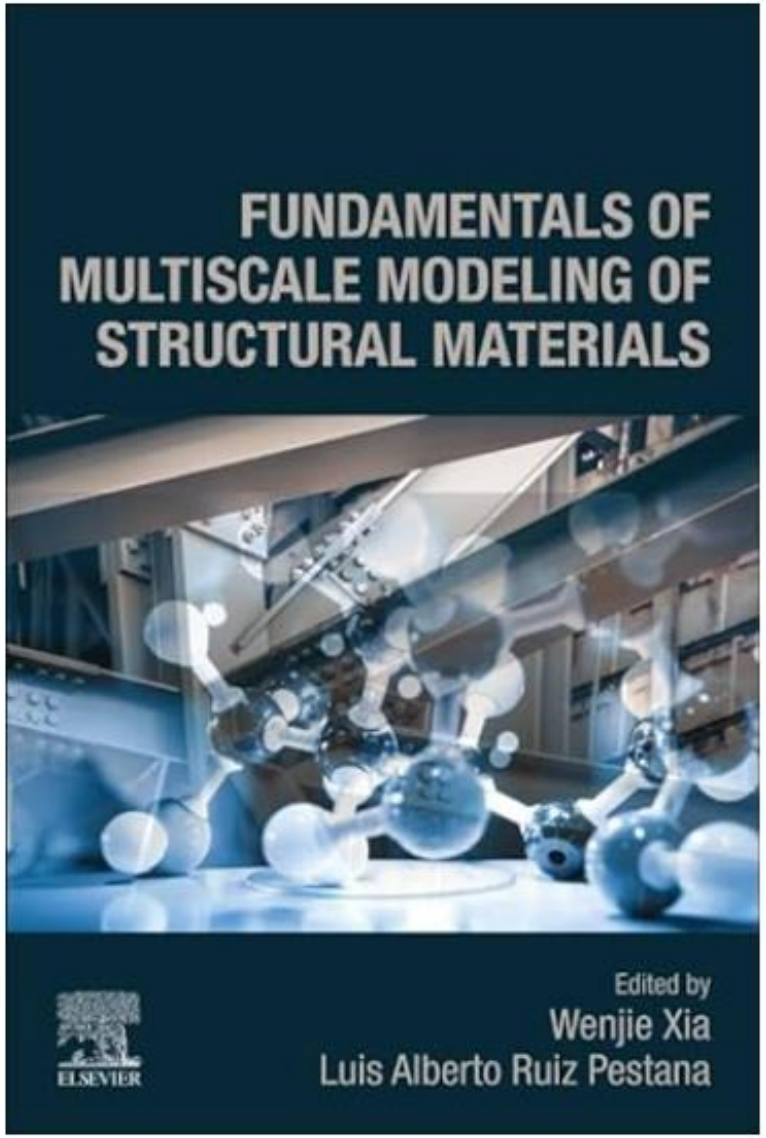
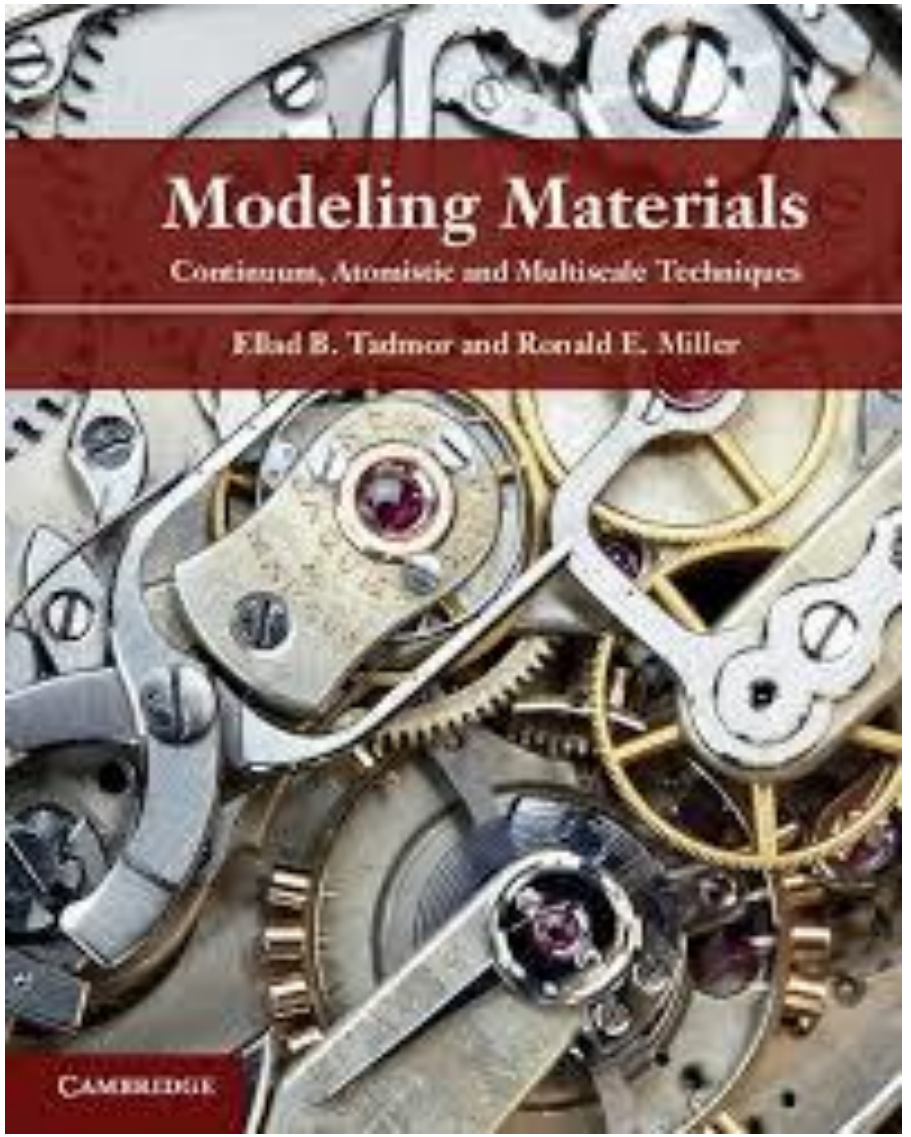
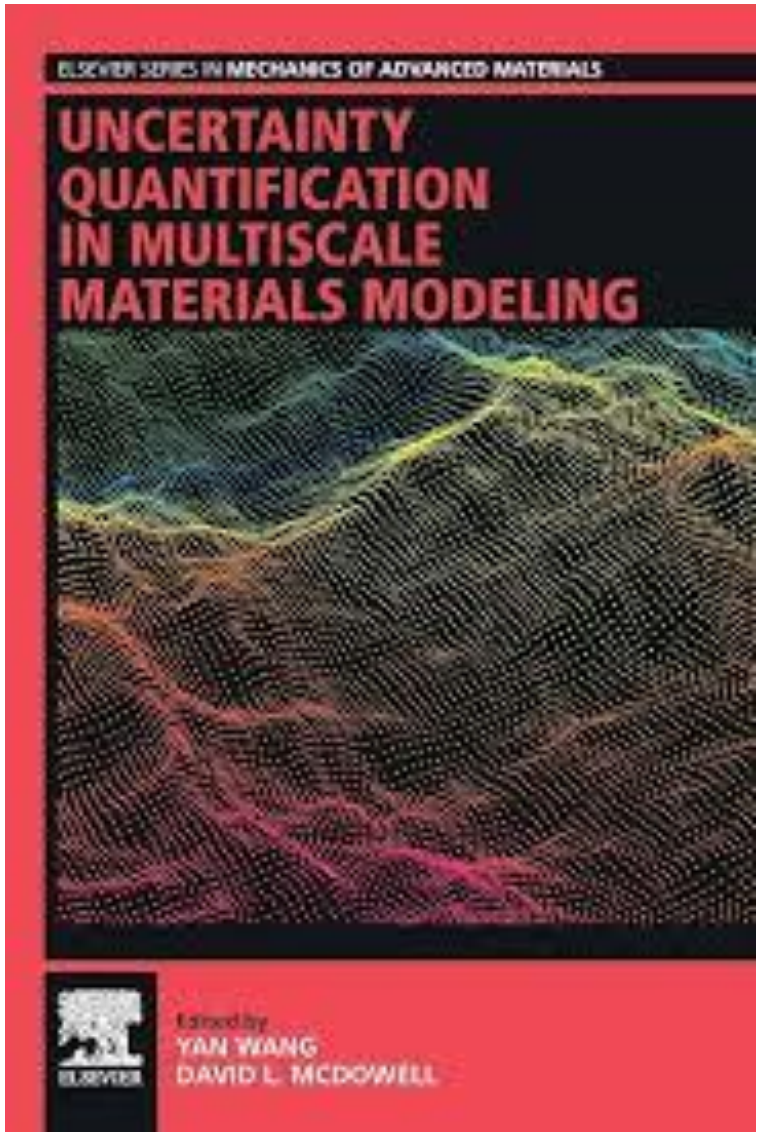


Fig. 1 Schematics of the multiscale modeling techniques across different time and length scales of material systems from quantum, all-atom, coarse-graining, mesoscale, to continuum. The paradigm shows the approximate ranges of time and length scales associated with each modeling technique along with relevant applications.

From book: Fundamentals of Multiscale Modeling of Structural Materials, Xia







https://www.sciencedirect.com/book/9780128230213/fundamentals-of-multiscale-modeling-of-structural-materials
https://www.cambridge.org/core/books/modeling-materials/7CC4027C34755637D8F641A0C8C26835#fndtn-information
https://www.sciencedirect.com/book/9780081029411/uncertainty-quantification-in-multiscale-materials-modeling

Programming and Programming Languages

Programming: Programming is the process of designing and building an executable computer program to accomplish a specific computing result or to perform a particular task.

Programming Languages: A programming language is a formal language comprising a set of instructions that produce various kinds of output. Programming languages are used in computer programming to implement algorithms.

Characteristics of Programming Languages

1.Syntax and Semantics: Every programming language has a unique set of rules for usage, known as its syntax (such as : after ***if*** statement in Python). Semantics refer to the meaning of different elements and expressions within the language's syntax (such as run a code when it meets ***if*** statement).

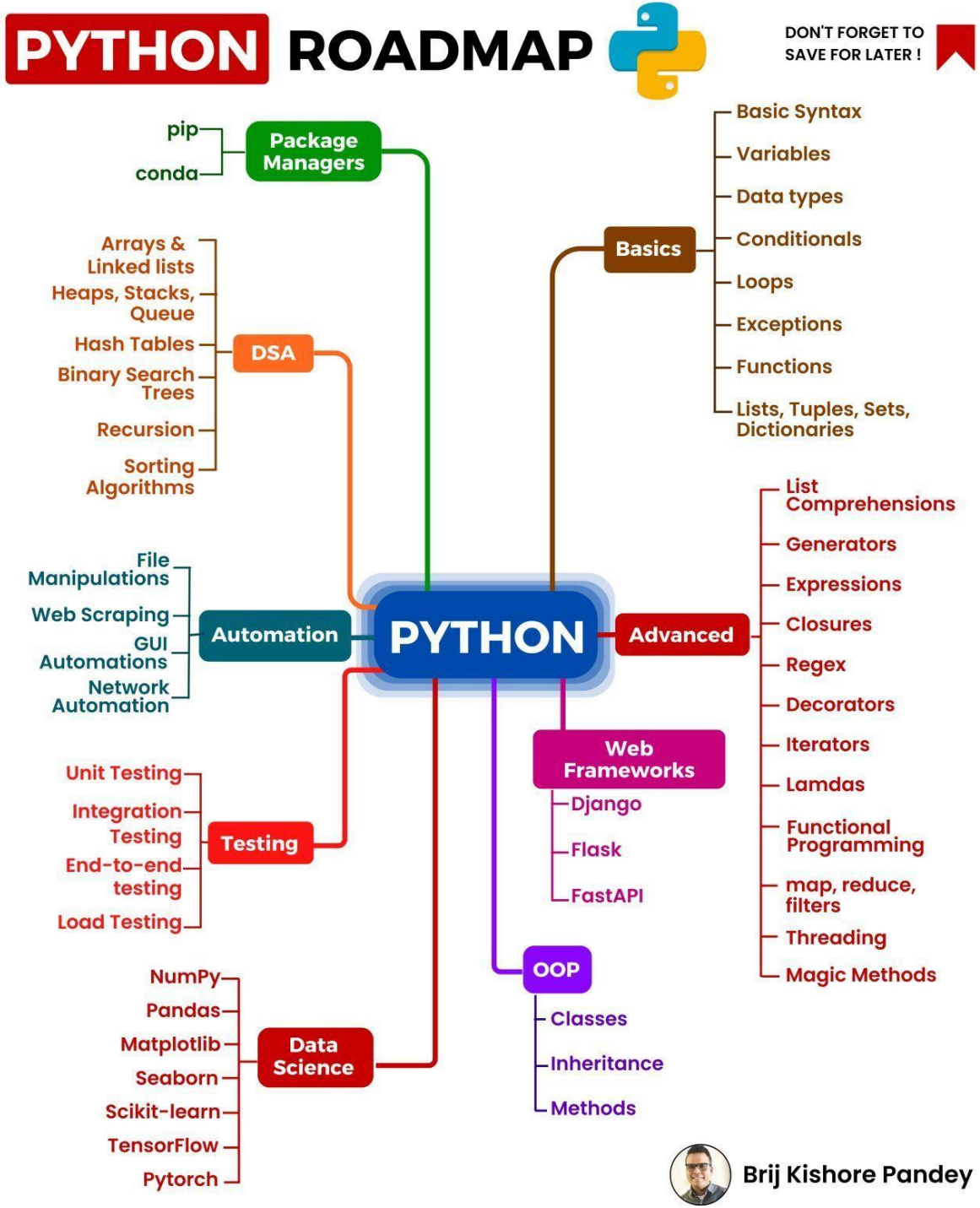
2.High-level and Low-level Languages: High-level languages (like Python, MATLAB, Java, and C#) are more abstract, and provide a syntax that is closer to human language. Low-level languages (like Assembly or C), in contrast are closer to machine code.

3.Static vs Dynamic Typing: Languages also differ in how they handle data types. In statically typed languages (e.g., C, Java), the type of a variable is known at compile time. In dynamically typed languages (e.g., Python, JavaScript), the type is determined at runtime which adds flexibility but reduces safety and performance.

4.Compiled vs Interpreted: Some languages are compiled, i.e., their programs are directly translated into machine-readable code (like C). Others are interpreted, i.e., their code is read and executed by a runtime program without prior conversion to machine code (like Python).

Programming and Programming Languages

Python


PYTHON ROADMAP
DON'T FORGET TO SAVE FOR LATER !
PYTHON
Package Managers
pip
conda
Basics
Basic Syntax
Variables
Data types
Conditionals
Loops
Exceptions
Functions
Lists, Tuples, Sets, Dictionaries
DSA
Arrays & Linked lists
Heaps, Stacks, Queue
Hash Tables
Binary Search Trees
Recursion
Sorting Algorithms
Automation
File Manipulations
Web Scraping
GUI Automations
Network Automation
Advanced
List Comprehensions
Generators
Expressions
Closures
Regex
Decorators
Iterators
Lamdas
Functional Programming
map, reduce, filters
Threading
Magic Methods
Web Frameworks
Django
Flask
FastAPI
Testing
Unit Testing
Integration Testing
End-to-end testing
Load Testing
OOP
Classes
Inheritance
Methods
Data Science
NumPy
Pandas
Matplotlib
Seaborn
Scikit-learn
TensorFlow
Pytorch
Brij Kishore Pandey

Data Structures

Variables: Variables are used to store individual data values. In a mechanical context, they could represent various physical properties or parameters.

```
# Variable to store the temperature of an engine (in degrees Celsius)
engine_temperature = 150

# Variable to store the speed of a rotating shaft (in RPM)
shaft_speed = 1200

print("Engine Temperature:", engine_temperature, "Celsius")
print("Shaft Speed:", shaft_speed, "RPM")
```

Arrays and Lists: An array is a collection of elements, useful for storing data elements of the same type. Lists are ordered collections of items that can be of different types. Lists are dynamic, meaning their size can change as elements are added or removed.

```
import numpy as np

# Using an array for numerical computation:
force_magnitudes = np.array([10, 20, 30, 40, 50])  # uniform data type (integers)
resultant_force = np.sum(force_magnitudes)  # easy to compute directly
print("Resultant Force:", resultant_force)

# Using a list for general data collection:
material_properties = ['steel', 7850, 210e9, {'ductility': 'high'}]  # mixed data types
print("Material Properties:", material_properties)
```

Data Structures

Sets: Sets are used for storing unique items.

```
# Set of unique component IDs in an assembly
component_ids = {'A1', 'A2', 'B1', 'A1'}  # 'A1' is duplicated

# Viewing the unique components
print("Unique component IDs:", component_ids)
```

Dictionaries: Dictionaries are key-value pairs and are useful for associating unique identifiers with specific data.

```
# Dictionary to store properties of different materials
material_properties = {
    'steel': {'density': 7850, 'young_modulus': 210e9},
    'aluminum': {'density': 2700, 'young_modulus': 69e9}
}

# Accessing properties of steel
print("Steel Properties:", material_properties['steel'])
```

Data Handling and Analysis

Reading and writing data files (CSV, Excel, JSON) using Python or MATLAB.

```
timestamp, sensor1, sensor2, sensor3
2024-05-01 00:00:00, 0.1, 0.3, 0.2
2024-05-01 00:00:01, 0.2, 0.4, 0.1
2024-05-01 00:00:02, 0.15, 0.35, 0.25
2024-05-01 00:00:03, 0.18, 0.38, 0.22
2024-05-01 00:00:04, 0.12, 0.32, 0.18
```

```
% Read data from a CSV file
data = readtable('validation.csv');

% Calculate the mean of the column 'sensor1'
sensor1_mean = mean(data.sensor1);

% Display the result
disp(['The mean of sensor1 is: ', num2str(sensor1_mean)]);
```

```
# pip install pandas matplotlib
import pandas as pd
import matplotlib.pyplot as plt
# Read data from a CSV file
data = pd.read_csv('validation.csv')
sensor1_mean = data['sensor1'].mean()
# Display the result
print(f'The mean of sensor1 is: {sensor1_mean}')
##############################################################################
# Parse 'timestamp' if it's in string format and you want to use it as X-axis
data['timestamp'] = pd.to_datetime(data['timestamp'])
# Plotting
plt.figure(figsize=(10, 6))  # Set the figure size for better readability
# Plot each sensor's data with a different line
plt.plot(data['timestamp'], data['sensor1'], label='Sensor 1', marker='o')
plt.plot(data['timestamp'], data['sensor2'], label='Sensor 2', marker='x')
plt.plot(data['timestamp'], data['sensor3'], label='Sensor 3', marker='s')
# Adding titles and labels
plt.title('Sensor Readings Over Time')
plt.xlabel('Timestamp')
plt.ylabel('Sensor Values')
plt.legend()  # Show legends
# Display the plot
plt.grid(True)  # Add grid for easier readability
plt.show()
```

Object-Oriented Programming (OOP) Concepts

Object-Oriented Programming (OOP) is a programming paradigm that uses "objects" - data structures consisting of data fields and methods together with their interactions - to design applications and computer programs. It centers around three main concepts: classes, objects, and inheritance.

Class: A blueprint for creating objects. A class defines a type in terms of its data (attributes) and its behavior (methods).
Object: An instance of a class. When a class is defined, no memory is allocated until an object is created from the class, also known as instantiation. Each object can hold different data, but they share the structure and behavior (methods) defined by their class.

```python
class MachineComponent:
    def __init__(self, material):
        self.material = material

    def display_material(self):
        print(f"Component material: {self.material}")

class Bearing(MachineComponent):  # Inherits from MachineComponent
    def __init__(self, material, bearing_type):
        super().__init__(material)
        self.bearing_type = bearing_type

    def display_info(self):
        print(f"Bearing type: {self.bearing_type}, Material: {self.material}")

# Creating an object of Bearing
bearing1 = Bearing('Ceramic', 'Ball')
bearing1.display_info()
```

Parallel and High-Performance Computing

Parallel Computing: Parallel computing involves dividing large problems into smaller ones, which are then solved concurrently across multiple processing elements within a computer. It can be based on CPUs or GPUs that perform the computations. Types:

1. **Data Parallelism**: Distributes chunks of data across multiple computing cores and performs the same operation on each chunk.
2. **Task Parallelism**: Distributes threads or tasks across different cores, where each task can be different.

High-Performance Computing (HPC) harnesses the power of parallel processing to run advanced application programs efficiently, reliably, and quickly. This often involves using supercomputers or computer clusters. Components:

1. **Supercomputers**: Extremely fast computers at the cutting edge of current processing capacity.
2. **Clusters**: Groups of linked computers that work together closely, so in many respects, they can be viewed as a single system.

Parallel Algorithms: Algorithms specifically designed to exploit parallel architectures.

Message Passing Interface (MPI): A standardized message-passing system to program parallel computers.

OpenMP (Open Multi-Processing): An API that supports multi-platform shared-memory parallel programming in C, C++, and Fortran.

CUDA (Compute Unified Device Architecture): A parallel computing platform and API model created by NVIDIA, allowing software developers to use a CUDA-enabled graphics processing unit (GPU) for general purpose processing.

SLURM/PBS schedulers: for submitting jobs in HPC

Parallel and High-Performance Computing

Serial Python Script for Factorial Computation

```python
import math
import time

def compute_factorial(number):
    result = math.factorial(number)
    print(f"The factorial of {number} is {result}")
    return result

def serial_factorial(numbers):
    results = []
    for number in numbers:
        results.append(compute_factorial(number))
    return results

if __name__ == '__main__':
    numbers = [5, 7, 9, 10, 12, 15, 18, 20]  # List of numbers to calculate factorial
    start_time = time.time()
    results = serial_factorial(numbers)
    end_time = time.time()
    #print("Factorial results:", results)
    print(f"Time taken for serial computation: {end_time - start_time} seconds")
```

Parallel Python Script for Factorial Computation

```python
from multiprocessing import Pool
import math
import time

def compute_factorial(number):
    return f"The factorial of {number} is {math.factorial(number)}"

def parallel_factorial(numbers):
    pool = Pool(processes=2)  # Creates a pool of 2 worker processes
    results = pool.map(compute_factorial, numbers)
    pool.close()  # No more tasks
    pool.join()   # Wait for completion
    return results

if __name__ == '__main__':
    numbers = [5, 7, 9, 10, 12, 15, 18, 20]
    start_time = time.time()
    results = parallel_factorial(numbers)
    end_time = time.time()
    for result in results:
        print(result)
    print(f"Time taken for parallel computation: {end_time - start_time} seconds")
    print("Number of CPUs:", multiprocessing.cpu_count())
```

Parallel and High-Performance Computing

```python
import numpy as np
import pycuda.autoinit
import pycuda.driver as drv
from pycuda.compiler import SourceModule
import time

def cpu_compute_squares(data):
    """ Compute squares using the CPU """
    return data**2
```

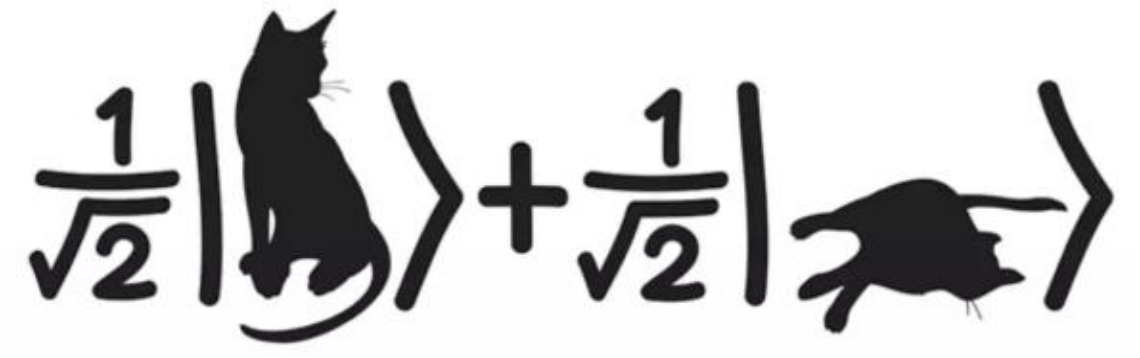
```python
def gpu_compute_squares(data):
    """ Compute squares using the GPU """
    mod = SourceModule("""
    __global__ void compute_squares(float *dest, float *a)
    {
        const int i = threadIdx.x + blockDim.x * blockIdx.x;
        dest[i] = a[i] * a[i];
    }
    """)
    compute_squares = mod.get_function("compute_squares")

    dest = np.empty_like(data)
    compute_squares(
        drv.Out(dest), drv.In(data),
        block=(1024, 1, 1), grid=(len(data) // 1024, 1)
    )
    return dest
```

```python
if __name__ == "__main__":
    # Generate large array of random floats
    data = np.random.randn(10000000).astype(np.float32)

    # Compute squares on CPU
    start_time = time.time()
    cpu_result = cpu_compute_squares(data)
    cpu_time = time.time() - start_time
    print("CPU computation time:", cpu_time)

    # Compute squares on GPU
    start_time = time.time()
    gpu_result = gpu_compute_squares(data)
    gpu_time = time.time() - start_time
    print("GPU computation time:", gpu_time)
```

What is Quantum Mechanics?

In classical mechanics, systems are defined as a deterministic collection of interacting particles whose positions and velocities evolve according to Newton's equations of motion.

In contrast, in quantum mechanics systems are described by a mathematical object known as the wavefunction, which depends on the positions of all the electrons and nuclei in the system. The wavefunction of the electron evolves over time according to the Schrödinger equation (Nobel prize in Physics 1933).



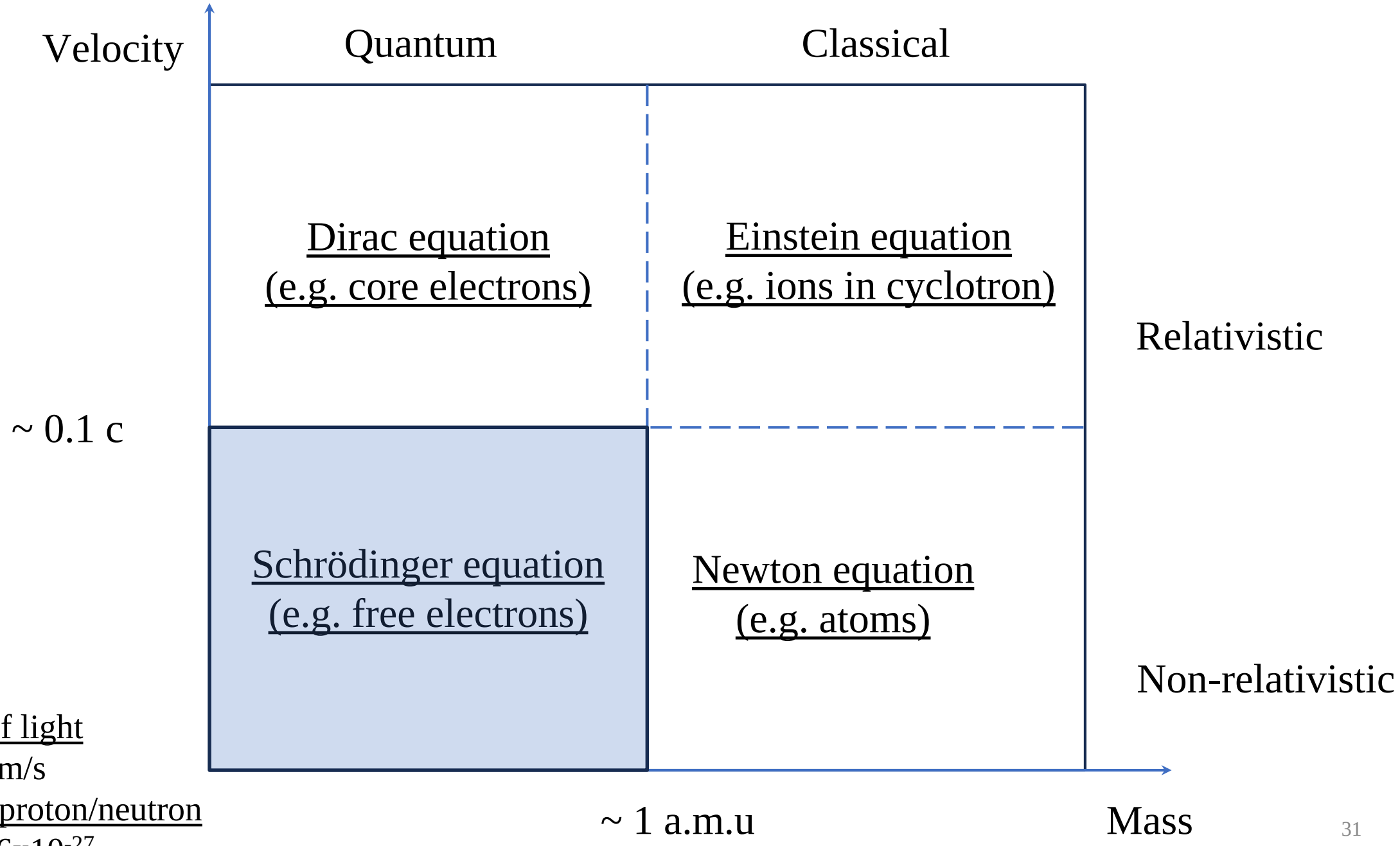
$$\hat{H}\,\Psi = E\,\Psi$$

Hamiltonian Operator (Energy operator)

Energy eigenvalue

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(\mathrm{r}) + V(r)\Psi(\mathrm{r}) = E\Psi(\mathrm{r})$$

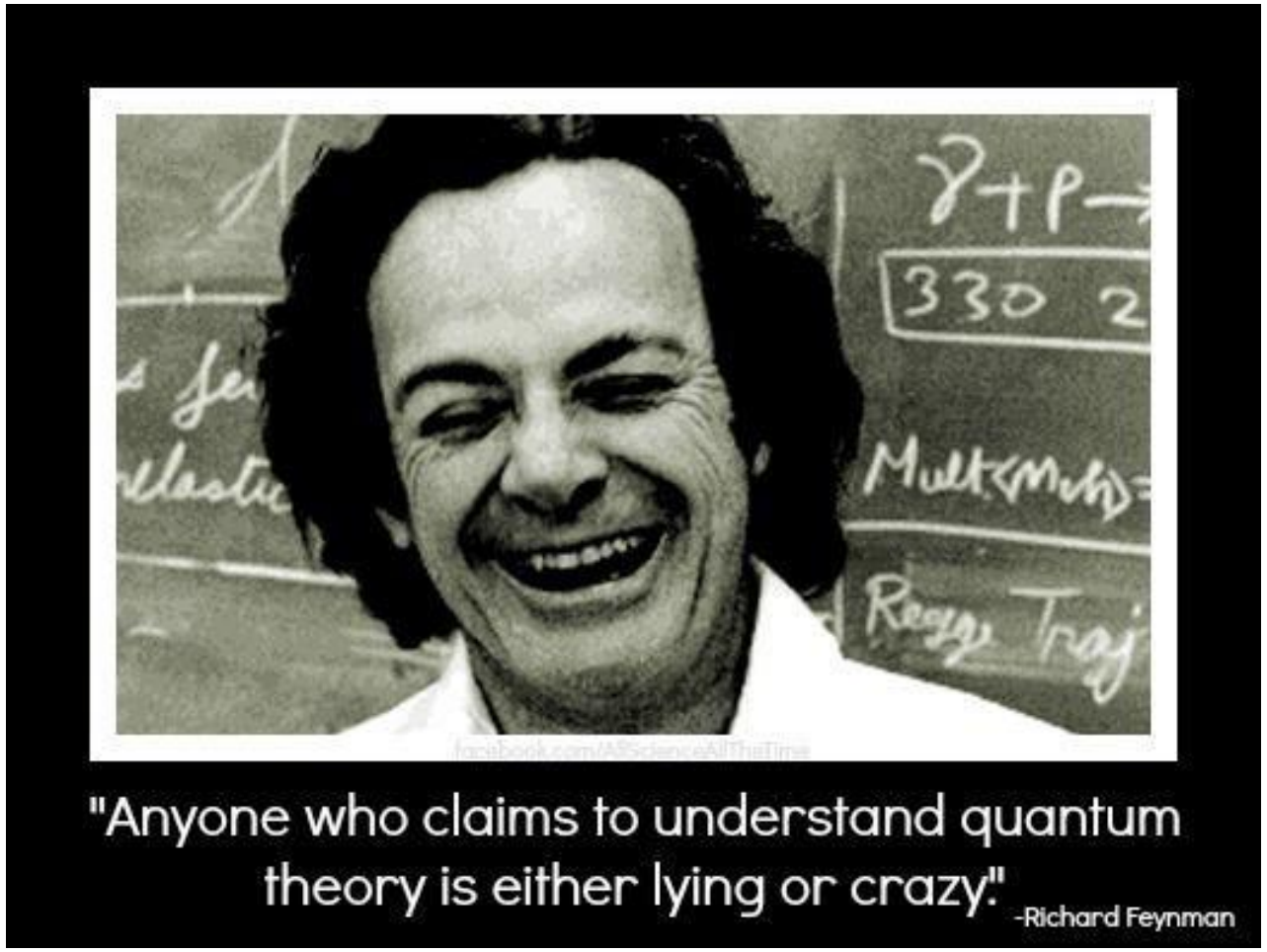
Kinetic Energy + *Potential Energy* = *Total Energy*



Velocity of light
$c = 3x10^{8}$ m/s

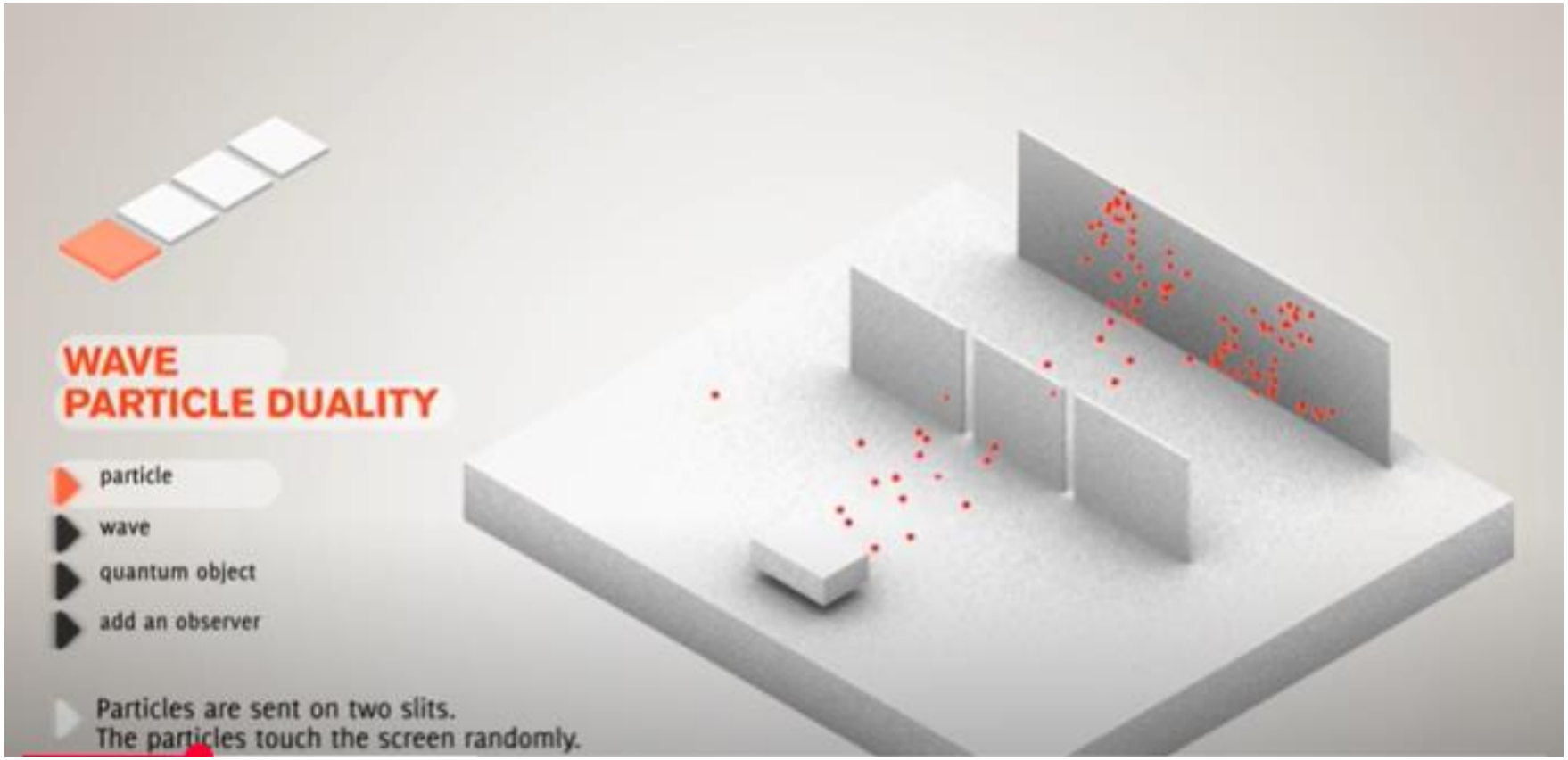
Mass of a proton/neutron
amu = $1.66x10^{-27}$

Quantum Mechanics is Difficult but Useful!



Key Principles of Quantum Mechanics

Wave-Particle Duality describes how every particle or quantum entity can exhibit both particle-like and wave-like behavior, e.g. in the double-slit experiment. Light behaves as a wave when it creates an interference pattern and as particles (photons) when detected individually. De Broglie wavelength $\lambda=hp$, λ is the wavelength, h is Planck's constant, p is particle's momentum.



https://youtu.be/qCmtegdqOOA

Introduction to Density Functional Theory

Many-body/electron solution of
Schrodinger equation is challenging → DFT

The Nobel Prize in Chemistry 1998

Photo from the Nobel Foundation archive.
Walter Kohn
Prize share: 1/2

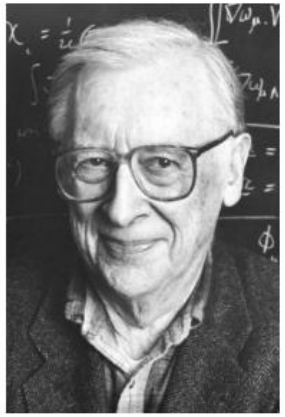


Photo from the Nobel Foundation archive.
John A. Pople
Prize share: 1/2

The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry"

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

P. HOHENBERG†
École Normale Superieure, Paris, France
AND
W. KOHN‡
École Normale Superieure, Paris, France and Faculté des Sciences, Orsay, France
and
University of California at San Diego, La Jolla, California
(Received 18 June 1964)

This paper deals with the ground state of an interacting electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the density, $F[n(\mathbf{r})]$, independent of $v(\mathbf{r})$, such that the expression $E\equiv\int v(\mathbf{r})n(\mathbf{r})d\mathbf{r}+F[n(\mathbf{r})]$ has as its minimum value the correct ground-state energy associated with $v(\mathbf{r})$. The functional $F[n(\mathbf{r})]$ is then discussed for two situations: (1) $n(\mathbf{r})=n_0+\tilde{n}(\mathbf{r})$, $\tilde{n}/n_0<<1$, and (2) $n(\mathbf{r})=\varphi(\mathbf{r}/r_0)$ with φ arbitrary and $r_0\to\infty$. In both cases F can be expressed entirely in terms of the correlation energy and linear and higher order electronic polarizabilities of a uniform electron gas. This approach also sheds some light on generalized Thomas-Fermi methods and their limitations. Some new extensions of these methods are presented.

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM
University of California, San Diego, La Jolla, California
(Received 21 June 1965)

From a theory of Hohenberg and Kohn, approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. (The exchange portion of our effective potential differs from that due to Slater by a factor of $\frac{2}{3}$.) Electronic systems at finite temperatures and in magnetic fields are also treated by similar methods. An appendix deals with a further correction for systems with short-wavelength density oscillations.

Introduction to Density Functional Theory

- Schrödinger equation for electrons: **wave–particle duality**,
- 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** vs **wavefunction** quantity

$$H\psi = E\psi$$

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

Exchange-correlation

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

Walter Kohn (2013)

- Although a **complete theory**, several approximations such as:

1) K-points, 2) vdW interactions, 3) kinetic energy deriv., 4) spin-orbit coupling, 5) e-ph coupling

(Convergence, OptB88vdW, TBmBJ, SOC topology, Superconducting prop.)

Many DFT databases with GGA-PBE, fixed k-point, no-SOC, …

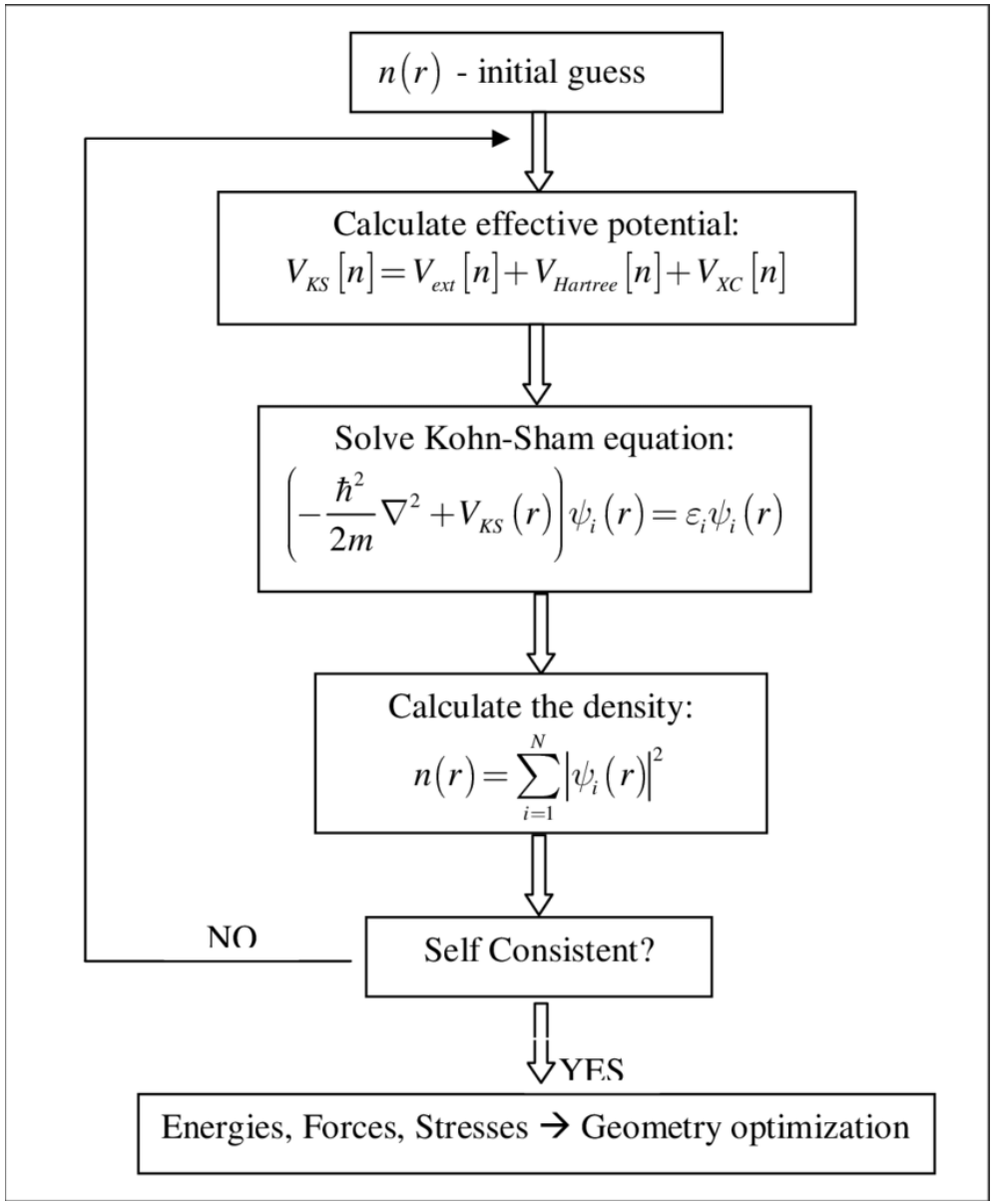
Exchange-correlation

The exchange-correlation functional aims to encapsulate all the many-body effects of a quantum system into a single term that can be added to the effective potential in which the electrons move.

1. **Exchange Interactions**: These arise due to the quantum mechanical principle that two electrons with the same spin cannot occupy the same spatial position, a consequence of the Pauli exclusion principle. This interaction results in a form of repulsion that is not purely electrostatic but quantum mechanical, influencing the spatial distribution of electrons with like spins.
2. **Correlation Interactions**: These describe how the motion of one electron in a system is correlated with the motion of all other electrons due to their mutual electrostatic interactions. Electrons tend to avoid each other due to these repulsive forces, which is not captured by considering only the average electron density or the exchange effects alone.

- **Approximations**: Various models and approximations are used to estimate Exc, the most common being:
  - **Local Density Approximation (LDA)**: Assumes the exchange-correlation energy per electron can be approximated by that of a uniform electron gas at each point in space.
  - **Generalized Gradient Approximation (GGA)**: Improves upon LDA by also considering the gradient of the electron density at each point, allowing for more accurate modeling of systems where the electron density changes rapidly.
  - **Hybrid Functionals**: Include a portion of exact exchange from Hartree-Fock theory combined with DFT exchange-correlation, providing better accuracy for some systems at the cost of increased computational effort.

Overview of the DFT Framework- 1D example




```python
import numpy as np
from scipy.linalg import eigh_tridiagonal
import matplotlib.pyplot as plt

def harmonic_potential(x):
    return 0.5 * (x ** 2)

def effective_potential(x, rho, alpha=0.5):
    """Combine external and Hartree potential"""
    V_ext = harmonic_potential(x)
    V_hartree = np.convolve(rho, np.exp(-alpha * np.abs(x)), mode='same') / alpha
    return V_ext + V_hartree
```

```python
def solve_kohn_sham(x, num_electrons):
    dx = x[1] - x[0]
    N = len(x)

    # Approximate second derivative using finite differences
    diagonal = np.full(N, -2.0 / dx**2)
    off_diagonal = np.full(N-1, 1.0 / dx**2)

    # Initial guess for electron density
    rho = np.ones(N) * (num_electrons / N)

    for _ in range(30):  # Self-consistent iterations
        V_eff = effective_potential(x, rho)

        # Hamiltonian matrix in tridiagonal form
        hamiltonian_diagonal = -0.5 * diagonal + V_eff

        # Solve the Schrodinger equation
        energies, psi = eigh_tridiagonal(hamiltonian_diagonal, off_diagonal, select='i', select_range=(0, num_electrons-1))

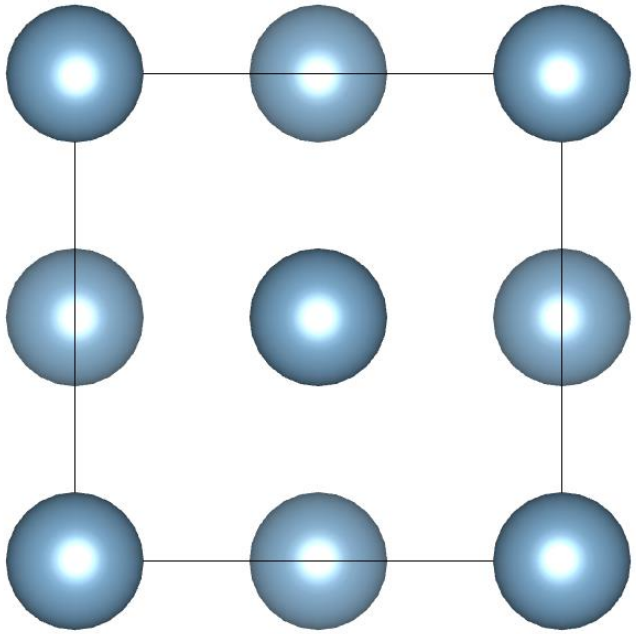
        # Update electron density
        rho_new = np.sum(psi**2, axis=1)
        rho = 0.7 * rho + 0.3 * rho_new  # Mixing to aid convergence

    return energies, psi, rho
```

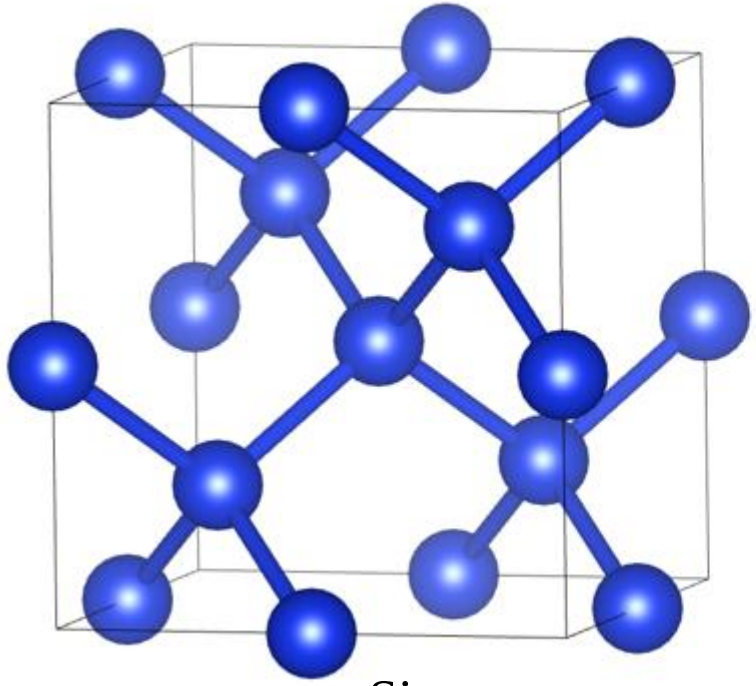
- Finite difference solution
- Single electron in a harmonic oscillator potential

Setting Up the System/Inputs

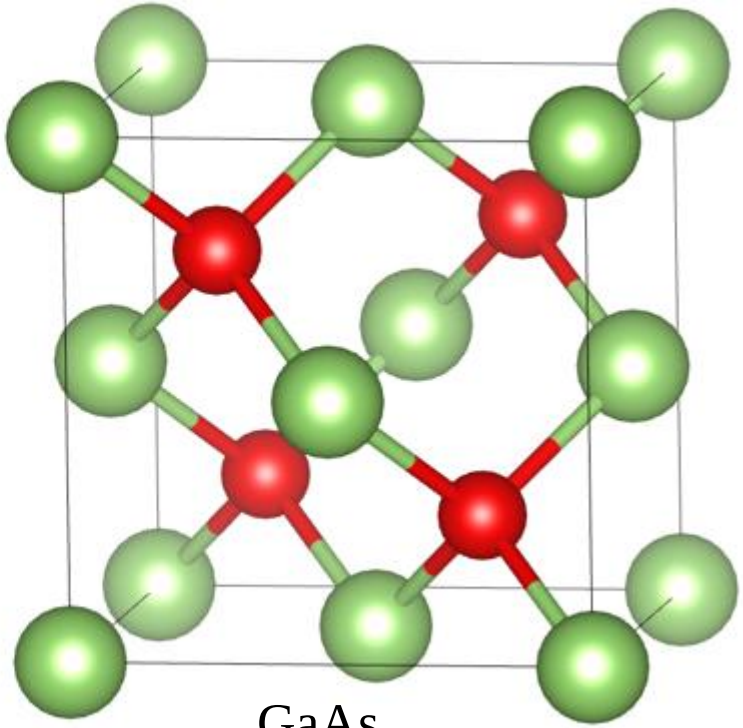
- Preparing the initial structure: atomic positions, lattice parameters
- These atomic positions can be obtained from experiments such as X-ray diffraction, NMR
- There are also large databases of such structures such as Crystallography Open Database, JARVIS-DFT, Materials Project, OQMD etc.
- Primitive (smallest) cells are preferred for atomistic simulations for computational cost reasons
- For defect/interface simulations large number of atoms could be necessary



Al



Si

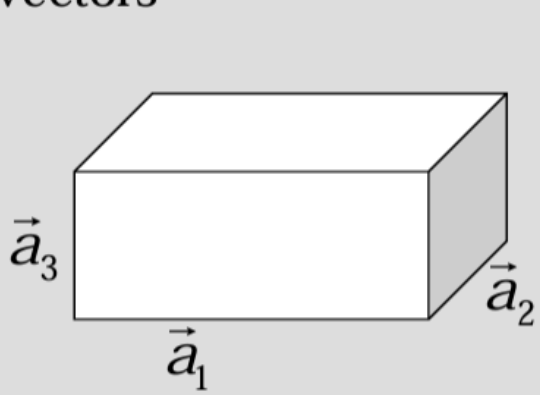


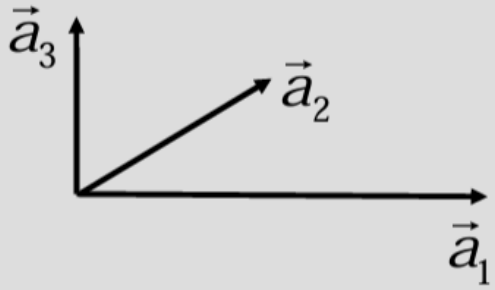
GaAs

Basis Sets

- In order to solve Kohn-Sham -equation, we need to expand the wavefunction in a basis set
- Simplify the problem of solving the Kohn-Sham equations by expanding the wavefunctions in a manageable set of basis functions.
- **Types**:
  - **Localized Orbitals**: Such as Gaussian or Slater-type orbitals; effective for molecular/isolated systems.
  - **Plane Waves**: used to model infinite systems, ideal for periodic systems; represent wave functions as sums of sinusoids. (Here a_1, a_2, a_3 are lattice vectors)

System is assumed to be placed inside a unit cell defined by the unit vectors





The volume of the unit cell is

$$\Omega = \left[\vec{a}_1, \vec{a}_2, \vec{a}_3\right] = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

$$\psi_i = \sum_\alpha c_\alpha \varphi_\alpha$$

Source: LANL

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\Omega}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\Omega}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\Omega}$$

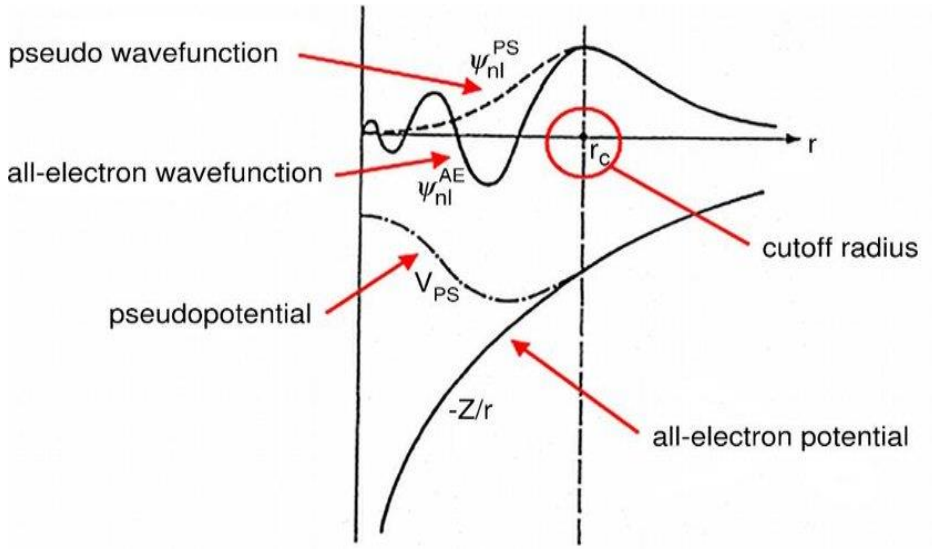
Reciprocal lattice vectors

Wave-vectors that satisfy the periodicity of the lattice

$$\vec{G}_{i_1 i_2 i_3} = \left(i_1 - \frac{N_1}{2}\right)\vec{b}_1 + \left(i_2 - \frac{N_2}{2}\right)\vec{b}_2 + \left(i_3 - \frac{N_3}{2}\right)\vec{b}_3$$

Pseudopotentials

- Effective potentials used to replace the all-electron potential near the nucleus in DFT calculations.
- Reduce computational complexity by focusing on valence electrons, effectively ignoring core electrons that do not participate in bonding
- **Types of Pseudopotentials**
  - **Norm-Conserving Pseudopotentials**: Ensure that the pseudowavefunction matches the all-electron wavefunction outside a certain cutoff radius.
  - **Ultrasoft Pseudopotentials**: Allow for greater flexibility and softer functions, reducing the plane wave basis set size needed for convergence.
  - **PAW (Projector Augmented Wave)**: A method that provides the accuracy of all-electron calculations with the efficiency of pseudopotentials.

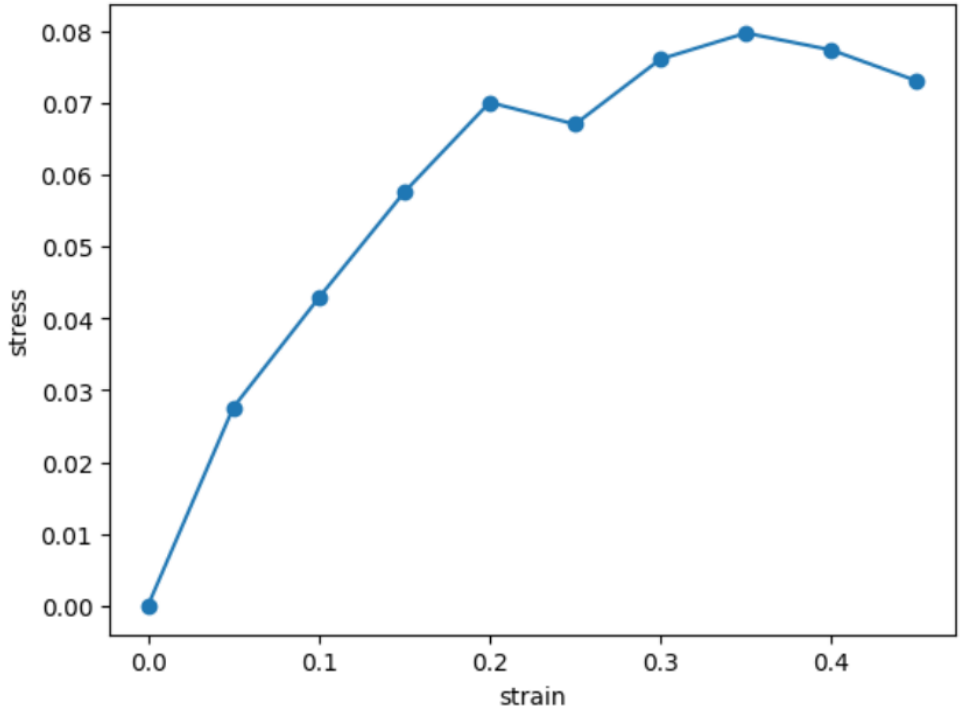


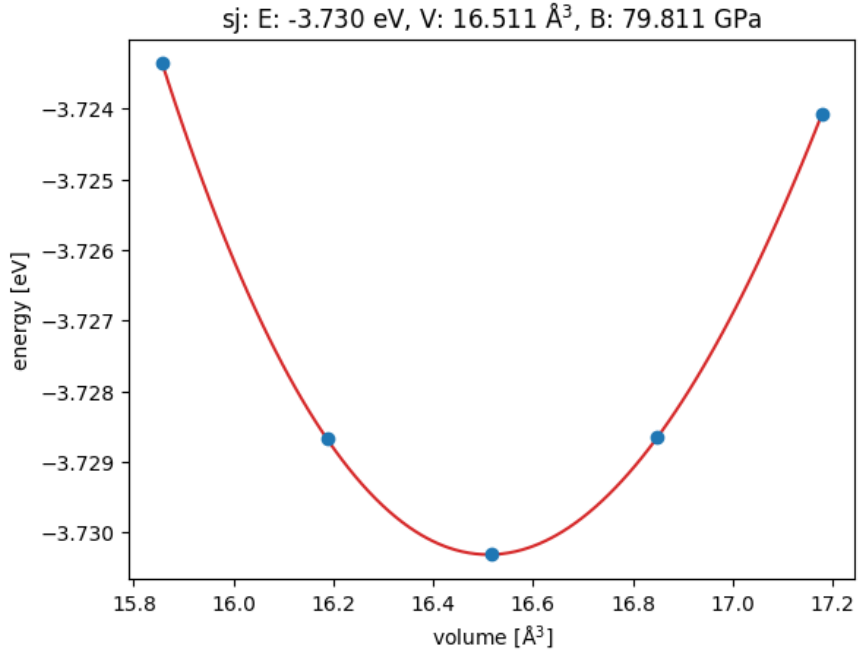
Choosing the Right Software

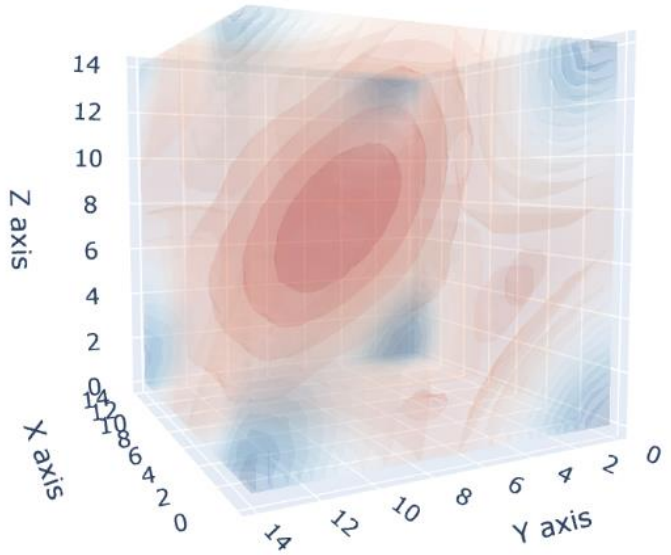
- Popular DFT software packages: VASP, Quantum ESPRESSO, GPAW, ABINIT
- Licensing and computational requirements
- Same Kohn-Sham equation, different format for input/output files
- Reading documentation could be useful

Outputs

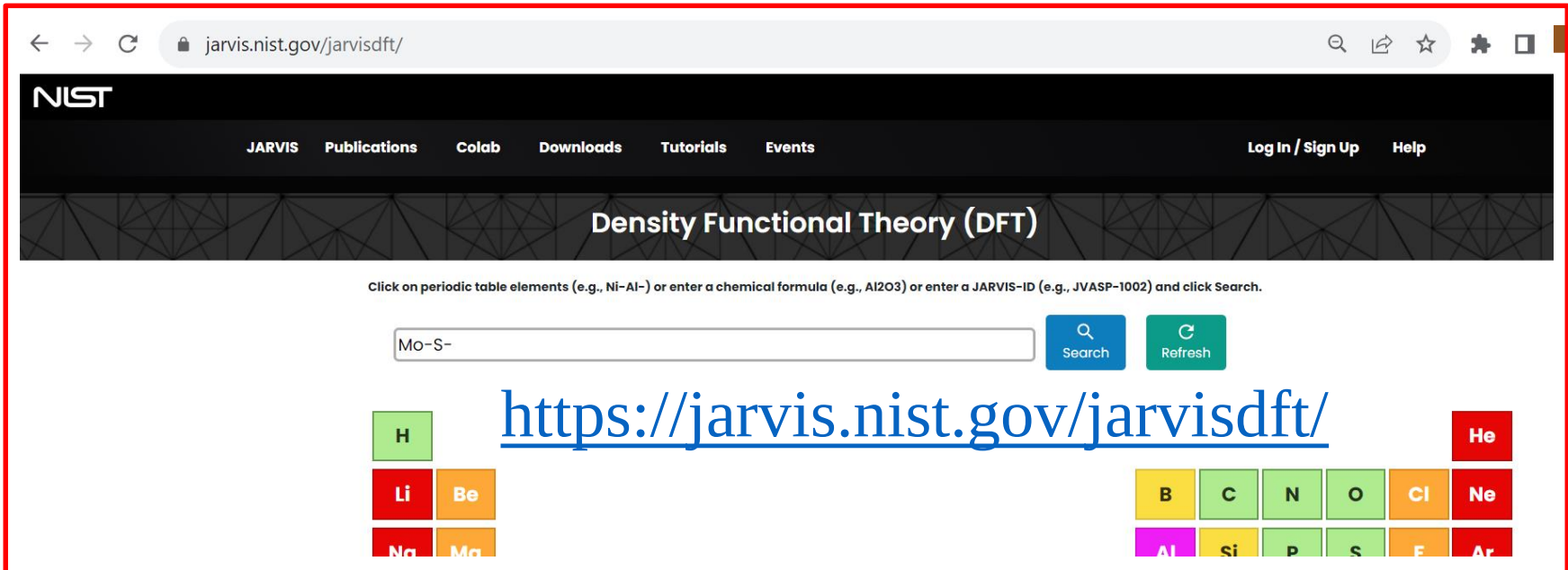
- Electronic density of states
- Charge density
- Optimized lattice constants
- Stress-strain curves
- Bulk modulus
- Elastic constants
- Thermal conductivity
- Electronic bandgap
- Magnetic moment
- Many more …..







JARVIS-DFT



https://jarvis.nist.gov/jarvisdft/

how 100 entries

Search:

id	formula	Spg	SpgNum	crys	func	E_form	OPT_gap	MBJ_gap	hse_gap	Kv	Gv	poisson	spillage	slme	mag	type
JVASP-664	MoS2	P-6m2	187	hexagonal	OptB88vdW	-0.88454	1.658	-	-	-	-	-	0.003	-	0.0	2D
JVASP-730	MoS2	R-3m	166	trigonal	OptB88vdW	-0.60967	0.000	-	-	-	-	-	0.976	-	-0.0	2D
JVASP-100856	MoS3	P2_1/m	11	monoclinic	OptB88vdW	-0.34773	0.443	-	-	-	-	-	-	-	0.0	3D
JVASP-111117	MoS2	P-3m1	164	trigonal	OptB88vdW	-0.69305	0.000	0.0	-	-	-	-	-	-	0.0	3D
JVASP-127507	MoS	Pm-3m	221	cubic	OptB88vdW	-0.18293	0.000	-	-	-	-	-	-	-	0.0	3D
JVASP-132473	MoS3I	P1	1	triclinic	OptB88vdW	0.06061	0.651	-	-	-	-	-	-	-	3.993	3D
JVASP-144515	Mo3S4	P-1	2	triclinic	OptB88vdW	-0.73826	0.000	-	-	-	-	-	-	-	0.0	3D
JVASP-228	MoS2	R-3m	166	trigonal	OptB88vdW	-0.69909	0.000	0.0	-	51.32	45.47	0.19	0.852	-	0.0	3D
JVASP-28379	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.95754	0.958	1.364	-	71.48	44.27	0.26	-	33.92	-	3D
JVASP-28413	MoS2	P-3m1	164	trigonal	OptB88vdW	-0.92268	1.207	1.471	-	-	-	-	-	32.7	0.0	3D
JVASP-28733	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.96160	0.921	-	-	70.62	47.69	0.23	0.013	-	0.0	3D
JVASP-34138	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.96135	0.920	1.356	-	-	-	-	-	33.93	0.0	3D

JARVIS-DFT

Features	JARVIS-DFT
#Materials (Struct., E_f, E_g)	80000
DFT functional/methods	vdW-DFT-OptB88, TBmBJ, DFT+SOC
K-point/cut-off	Converged for each material
SCF convergence criteria	Energy & Forces
Elastic tensors & point phonos	17402
Piezoelectric, IR spect.	4801
Dielectric tensors (w/o ion)	4801 (15860)
Electric field gradients	11865
SuperCon Tc	2200 (1058 ambient condition)

Features	JARVIS-DFT
2D monolayers	1011
Raman spectra	400
Seebeck, Power Factors	23210
Solar SLME	8614
Spin-orbit Coupling Spillage	11383
WannierTB	1771
STM images	1432
Surfaces	300
Defects	400
Interfaces	1.4 trillion (IU), 600 (ASJ)

JARVIS-DFT

High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory

Kamal Choudhary, Irina Kalish, Ryan Beams & Francesca Tavazza

Scientific Reports **7**, Article number: 5179 (2017) | Cite this article

Computational screening of high-performance optoelectronic materials using OptB88vdW and TB-mBJ formalisms

Kamal Choudhary, Qin Zhang, Andrew C.E. Reid, Sugata Chowdhury, Nhan Van Nguyen, Zachary Trau
Marcus W. Newrock, Faical Yannick Congo & Francesca Tavazza

Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods

Kamal Choudhary*, Marnik Bercx, Jie Jiang, Ruth Pachter, Dirk Lamoen, and Francesca Tavazza

Cite this: *Chem. Mater.* 2019, 31, 15, 5900−5908
Publication Date: July 17, 2019
https://doi.org/10.1021/acs.chemmater.9b02166

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Kamal Choudhary, Kevin F. Garrity, Vinit Sharma, Adam J. Biacchi, Angela R. Hight Walker & Francesca Tavazza

npj Computational Materials **6**, Article number: 64 (2020) | Cite this article

Data-driven discovery of 3D and 2D thermoelectric materials

Kamal Choudhary[2,1], Kevin F Garrity[1] and Francesca Tavazza[1]

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Citation Kamal Choudhary *et al* 2020 *J. Phys.: Condens. Matter* **32** 475501

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High-Throughput DFT-Based Discovery of Next Generation Two-Dimensional (2D) Superconductors

Daniel Wines*, Kamal Choudhary, Adam J. Biacchi, Kevin F. Garrity, and Francesca Tavazza

Cite this: *Nano Lett.* 2023, 23, 3, 969−978
Publication Date: January 30, 2023
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Predicting anomalous quantum confinement effect in van der Waals materials

Kamal Choudhary and Francesca Tavazza
Phys. Rev. Materials **5**, 054602 – Published 7 May 2021

DOI: 10.1039/D4DD00031E (Paper) *Digital Discovery*, 2024, Advance Article

InterMat: accelerating band offset prediction in semiconductor interfaces with DFT and deep learning†

Kamal Choudhary * and Kevin F. Garrity

Can a deep-learning model make fast predictions of vacancy formation in diverse materials?

Kamal Choudhary; Bobby G. Sumpter

Check for updates

+ Author & Article Information

AIP Advances 13, 095109 (2023)

What is Classical Mechanics?

- **Definition:**
  - Study of the motion of bodies in a frame of reference
  - Deals with macroscopic scales and speeds much lower than the speed of light
- **Applications:**
  - Predicting planetary motions
  - Designing mechanical systems (e.g., vehicles, machinery)
  - Understanding structural dynamics
- **Limitations:**
  - Not applicable at atomic scales or near-light speeds
  - Replaced by quantum mechanics and relativity in such cases

Introduction to Molecular Dynamics

- **What is molecular dynamics (MD)?**

Numerical method for studying many-particle systems such as molecules, clusters, and even macroscopic systems such as gases, liquids and solids

- **First reported MD simulation:**

  Alder + Wainwright (1957): Phase diagram of a hard-sphere gas

- **Basic idea of molecular dynamics:**

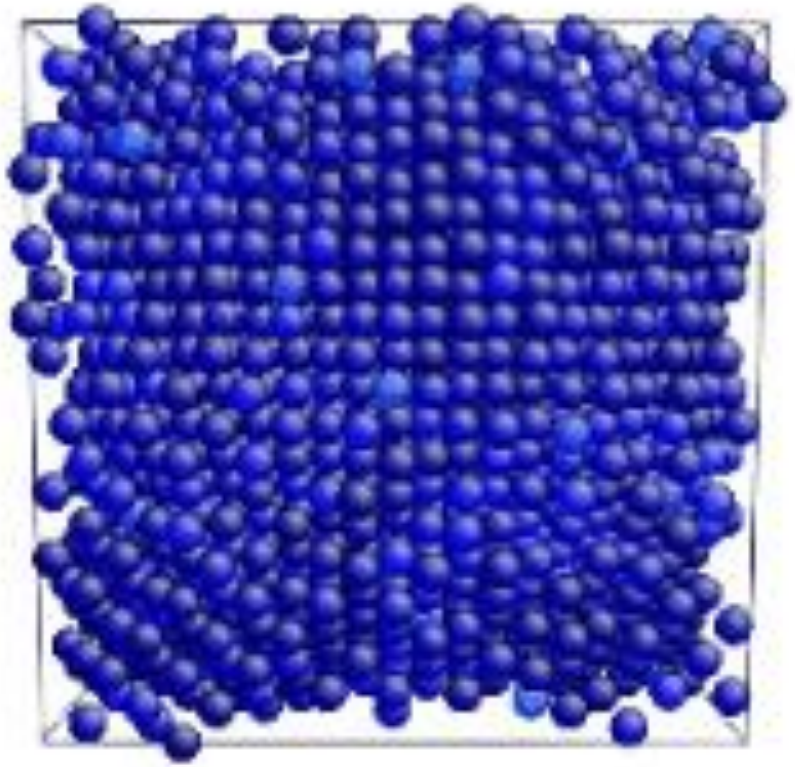
  Solution of Newton's equations of motion for the individual partic (atoms, ions, …)

  Interactions are approximated by classical **model potentials** constructed by comparison with experiment (empirical potentials)

  Leads to simulation of purely classical many-particle problem

- **Example:**

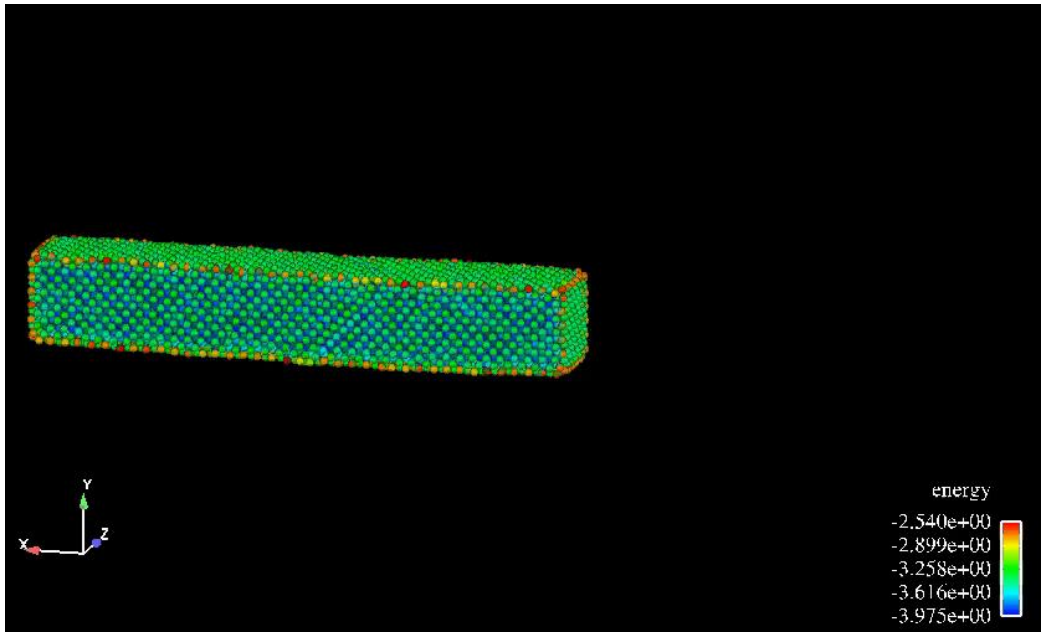
  Tensile Loading of an Aluminum Single Crystal



Movie showing deformation of single crystal aluminum loaded in the <100> direction at a strain rate of 10^{10} s^{-1} and a temperature of 300 K.
https://www.cavs.msstate.edu/icme/code/lammps/tutorials/lammps/uniaxial_tension.php

Overview of MD

- Pick atoms/particles, masses and forces (or potential) **fitted to DFT**/experiments
- Initialize positions and momentum (boundary conditions in space and time)
- Solve **F** = m **a** to determine **r**(t), **v**(t), **the integrator**, and note time is discrete (t_k) not continuous
- Compute properties along the trajectory
- Estimate errors
- Try to use the simulation to answer physical questions



Phase Transition for a Hard Sphere System

B. J. Alder and T. E. Wainwright
University of California Radiation Laboratory, Livermore, California
(Received August 12, 1957)

A CALCULATION of molecular dynamic motion has been designed principally to study the relaxations accompanying various nonequilibrium phenomena. The method consists of solving exactly (to the number of significant figures carried) the simultaneous classical equations of motion of several hundred particles by means of fast electronic computors. Some of the details as they relate to hard spheres and to particles having square well potentials of attraction have been described.[1,2] The method has been used also to calculate equilibrium properties, particularly the equation of state of hard spheres where differences with previous Monte Carlo[3] results appeared.

Alder & Wainwright, J Chem. Phys. ***27****, 1208 (1957).*

Interatomic Potentials and Force Fields

Interatomic potentials are **mathematical functions** that describe the potential energy between atoms or molecules as a **function of their positions**. These potentials are crucial for determining the forces in an MD simulation.

Types of Force Fields (FFs)

- **Pairwise Potentials**: **Simplest form**, considering only interactions between pairs of atoms. Examples include Lennard-Jones and Coulombic potentials.
- **Many-Body Potentials**: Consider interactions among **three or more atoms simultaneously**, providing a more accurate representation of atomic interactions. Examples include Embedded Atom Method (EAM) and Tersoff potentials.
- **Bonded Potentials**: Used for molecules, accounting for bond stretching, angle bending, and torsional interactions.

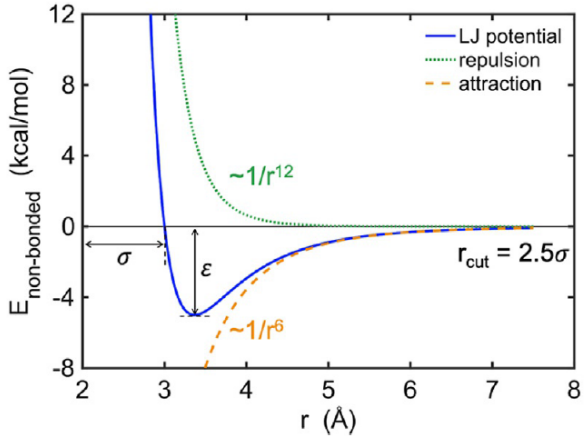


Fig. 5 The Lennard-Jones (LJ) potential. In the figure, r is the distance between a pair of atoms, r_{cut} is the cutoff distance, 2.5σ is a typical value, ε is the depth of the minimum energy, and σ is a length scale parameter related to the equilibrium distance between atoms. The *dotted and dashed lines* show the repulsion and attraction branches of the LJ potential, respectively.

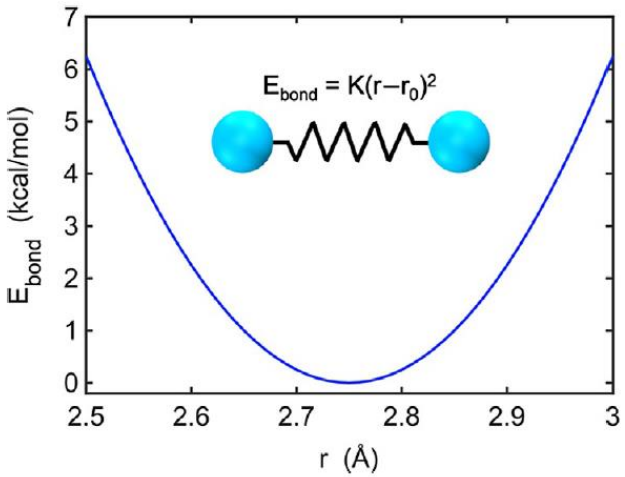


Fig. 3 Harmonic potential, $E_{bond}(r) = K(r - r_0)^2$, where $K = 100$ kcal/mol/Å^2 is the bond spring constant, and $r_0 = 2.75$ Å is the equilibrium bond length.

Types of FF

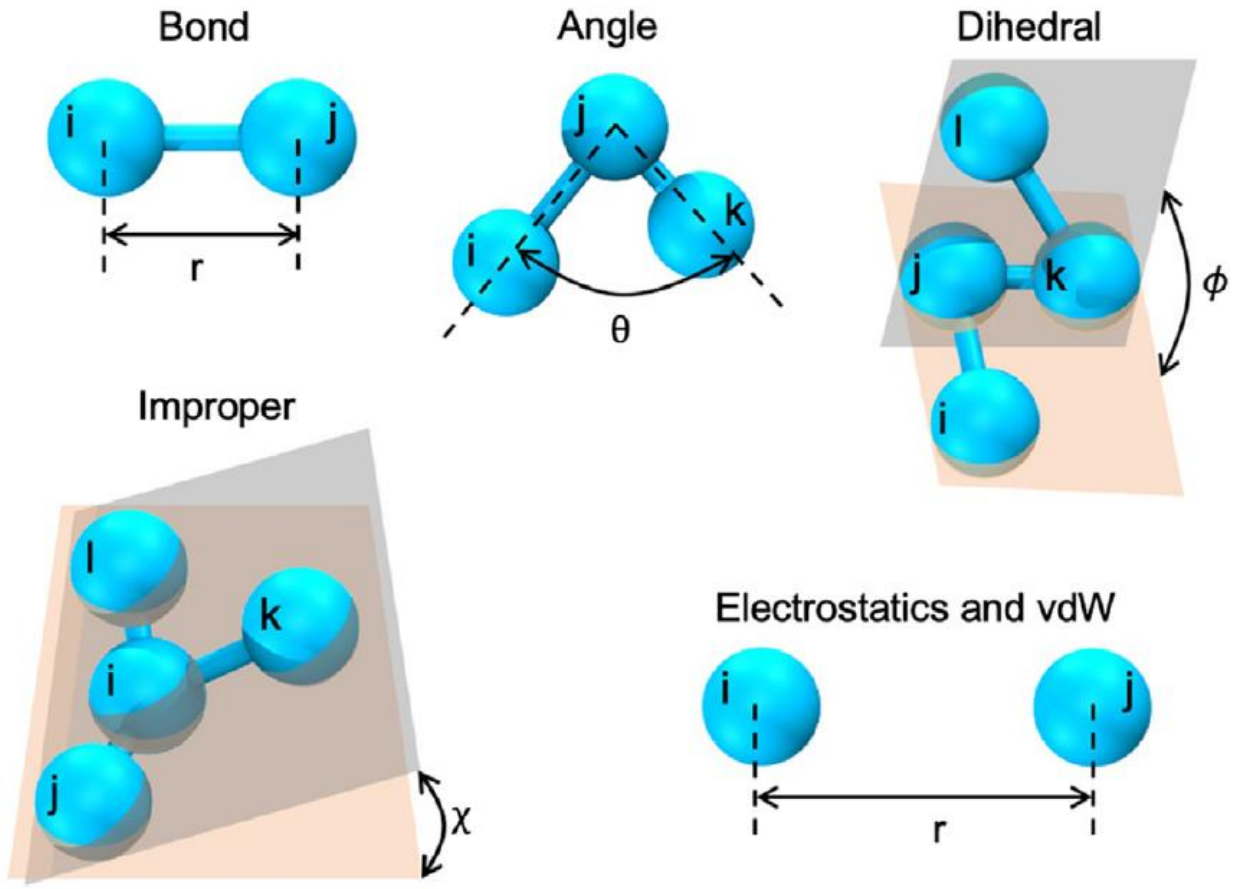


Fig. 2 Different types of interactions typically included in empirical force fields. Bond, angle, dihedral, and improper interactions are considered bonded, and electrostatics and van der Waals nonbonded.

From book: Fundamentals of Multiscale Modeling of Structural Materials, Xia

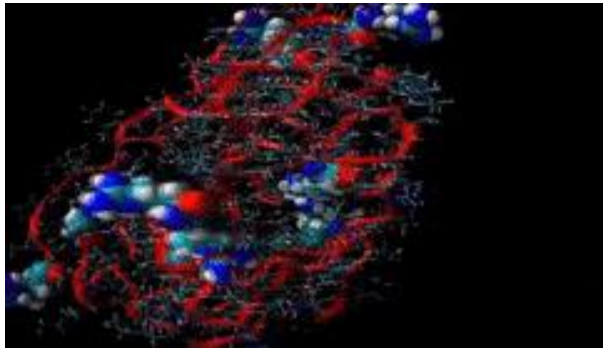
Table 1 List of commonly used force fields in MD or MC simulations.

Force field family	Variants	Most applicable system
CHARMM [1]	CGenFF, CHARMM22, CHARMM27, and CHARMM36.	Organic molecules, solutions, polymers, biochemical molecules, etc.
AMBER [2]	GAFF, GLYCAM, ff94, ff96, ff98, ff99, ff02, ff02EP, etc.	Biochemical molecules (proteins, nucleic acids, polysaccharides, etc.)
DREIDING [15]	–	Organic, biological, polymeric, and main-group inorganic molecules
OPLS [3,4]	OPLS-AA and OPLS-UA.	Biological macromolecules, solutions, etc.
MMX [9,10]	MM2, MM3, MM4, MM +, etc.	Organic chemical compounds, free radicals, ions, etc.
CFF [14]	COMPASS, COMPASS II, CFF95, CFF91, and PCFF.	Organic small molecules, biomolecules, molecular sieves, polymers, metals, etc.
ReaxFF [16]	–	Metals, ceramics, silicon, polymers
ClayFF [17]	–	Hydrated and multicomponent mineral systems and their interfaces with aqueous solutions.

Classical Force-Fields

One parameter to fit/optimize

- Coulomb potential $V(q_1(\vec{r}_1), q_2(\vec{r}_2)) = \frac{kq_1q_2}{|\vec{r}_2 - \vec{r}_1|}$
- Lennard-Jones potential $V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$
- 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

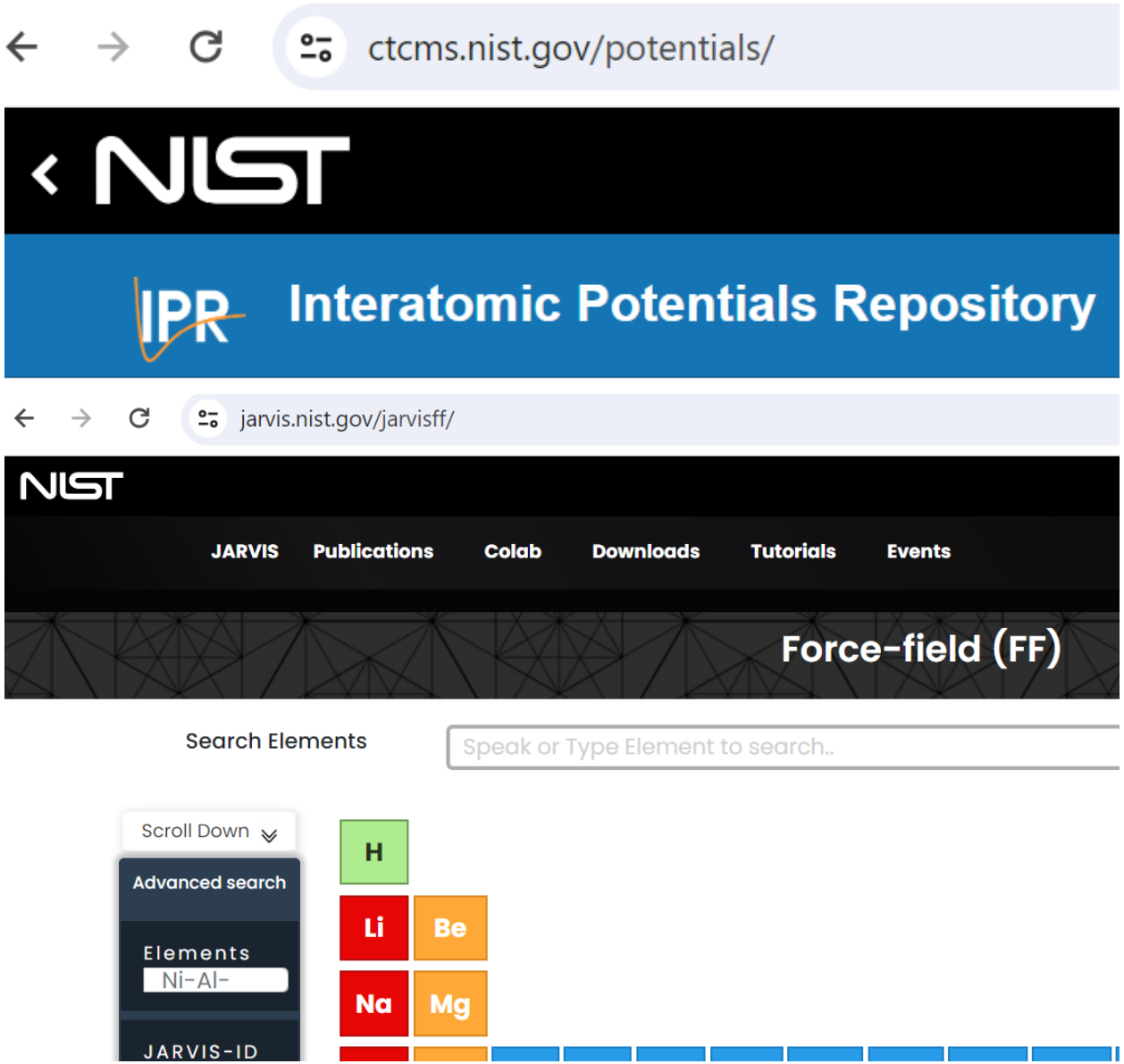
- Fixed charge potentials: Coulomb-Buckingham
- Other FFs: ReaxFF, COMB, AMBER, CHARMM, OPLS etc.

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

Berni Alder

Email: kamal.choudhary@nist.gov

JARVIS-FF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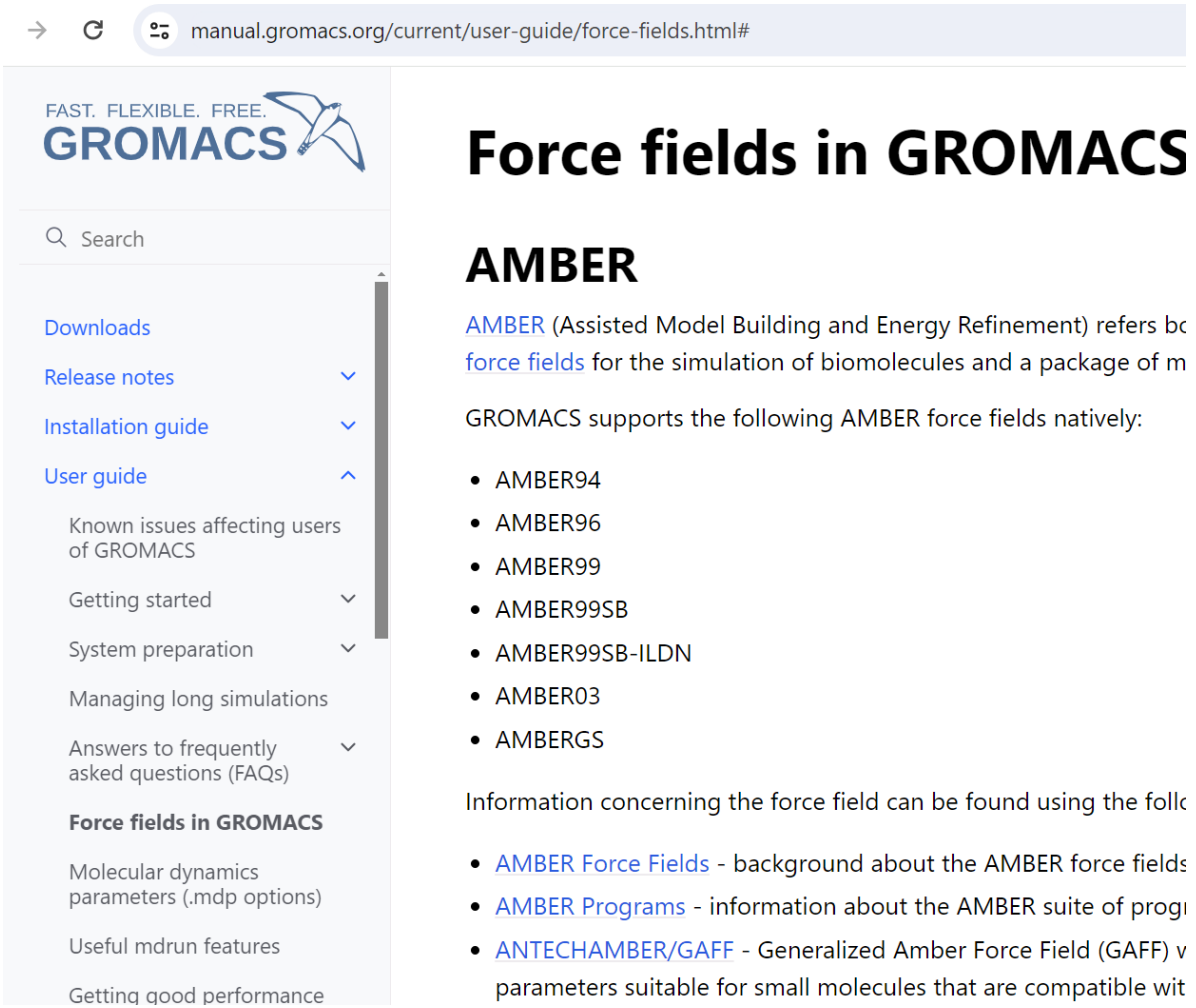
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AMBER99SB-ILDN
AMBER03
AMBERGS
Information concerning the force field can be found using the follc
AMBER Force Fields - background about the AMBER force fields
AMBER Programs - information about the AMBER suite of progr
ANTECHAMBER/GAFF - Generalized Amber Force Field (GAFF) v
parameters suitable for small molecules that are compatible wit

Statistical Ensembles

Real-world experiments often operate under **specific conditions** (constant temperature, pressure, volume, etc.)

Statistical ensembles (hypothetical copies) allow us to relate the multitude of possible microstates ((e.g., Avogadro's number, 10^{23}) to macroscopic thermodynamic quantities by **averaging over all microstates** according to certain probabilities

Ways to describe a system of particles with specific constraints and conditions:

- **Microcanonical Ensemble (NVE):** Fixed N, V, E
- **Canonical Ensemble (NVT):** Fixed N, V, T
- **Grand Canonical Ensemble (μVT):** Fixed μ, V, T
- **Isothermal-Isobaric Ensemble (NPT):** Fixed N, P, T

Number of particles (N), Chemical potential (μ), Volume (V), Pressure (P), Temperature (T)

Overcoming Challenges

- **Hybrid Approaches:** Combining classical force fields with **quantum mechanical** methods (QM/MM) to accurately model systems where electronic effects are non-negligible.
- **Development of New Force Fields:** Ongoing research into more versatile and robust force fields that can handle a broader range of interactions and conditions such as **Machine Learning Force-Fields**.

Martin Karplus Facts

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Martin Karplus
The Nobel Prize in Chemistry 2013

Born: 15 March 1930, Vienna, Austria

Affiliation at the time of the award: Université de Strasbourg, Strasbourg, France; Harvard University, Cambridge, MA, USA

Prize motivation: "for the development of multiscale models for complex chemical systems"

Prize share: 1/3

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Cite this: *Digital Discovery*, 2023, **2**, 346

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]

Classical force fields (FFs) based on machine learning (ML) methods show great potential for large scale simulations of solids. MLFFs have hitherto largely been designed and fitted for specific systems and are not usually transferable to chemistries beyond the specific training set. We develop a unified atomisitic line graph neural network-based FF (ALIGNN-FF) that can model both structurally and chemically diverse solids with any combination of 89 elements from the periodic table. To train the ALIGNN-FF model, we use the JARVIS-DFT dataset which contains around 75 000 materials and 4 million energy-force entries, out of which 307 113 are used in the training. We demonstrate the applicability of this method for fast optimization of atomic structures in the crystallography open database and by predicting accurate crystal structures using a genetic algorithm for alloys.

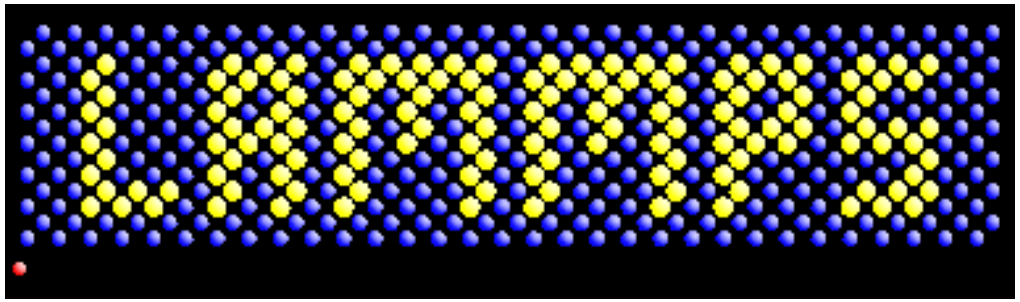
Received 12th September 2022
Accepted 12th January 2023

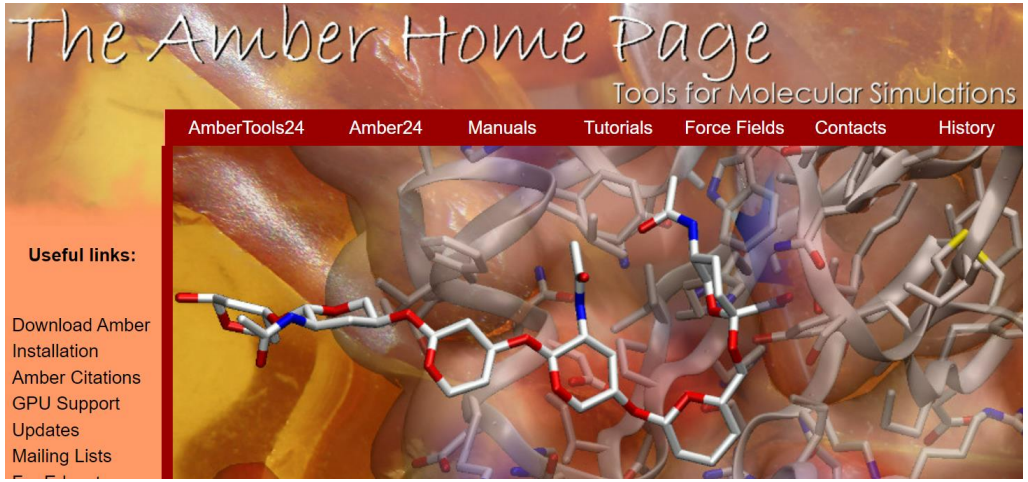
DOI: 10.1039/d2dd00096b

rsc.li/digitaldiscovery

Choosing the Right Software

- Popular MD software packages: LAMMPS, GROMACS, AMBER, CHARMM, OpenMM
- Choose based on available force-fields/implementations
- Same Newton's equation, different format for input/output files
- Reading documentation could be useful





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What is Continuum Mechanics?

Key Areas of Study

- **Elasticity**: Behavior of materials that return to their original shape after deformation when external forces are removed.
- **Plasticity**: Behavior of materials that undergo permanent deformation under external forces.
- **Viscoelasticity**: Materials exhibit both viscous (material's resistance to flow) and elastic characteristics when undergoing deformation.

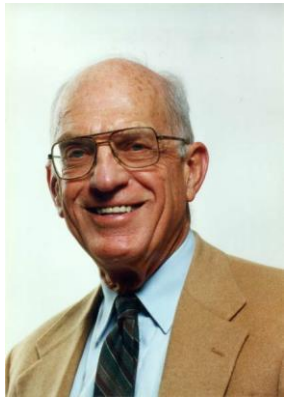
Governing Equations

- **Conservation of Mass**
- **Conservation of Momentum**
- **Conservation of Energy**

Applications

- Predicting the effects of stress and strain on structures and materials.
- Designing materials and structures in civil, aerospace, automotive, and mechanical engineering.
- Understanding geological phenomena and biomaterial behaviors

What is Finite Element Method (FEM)?



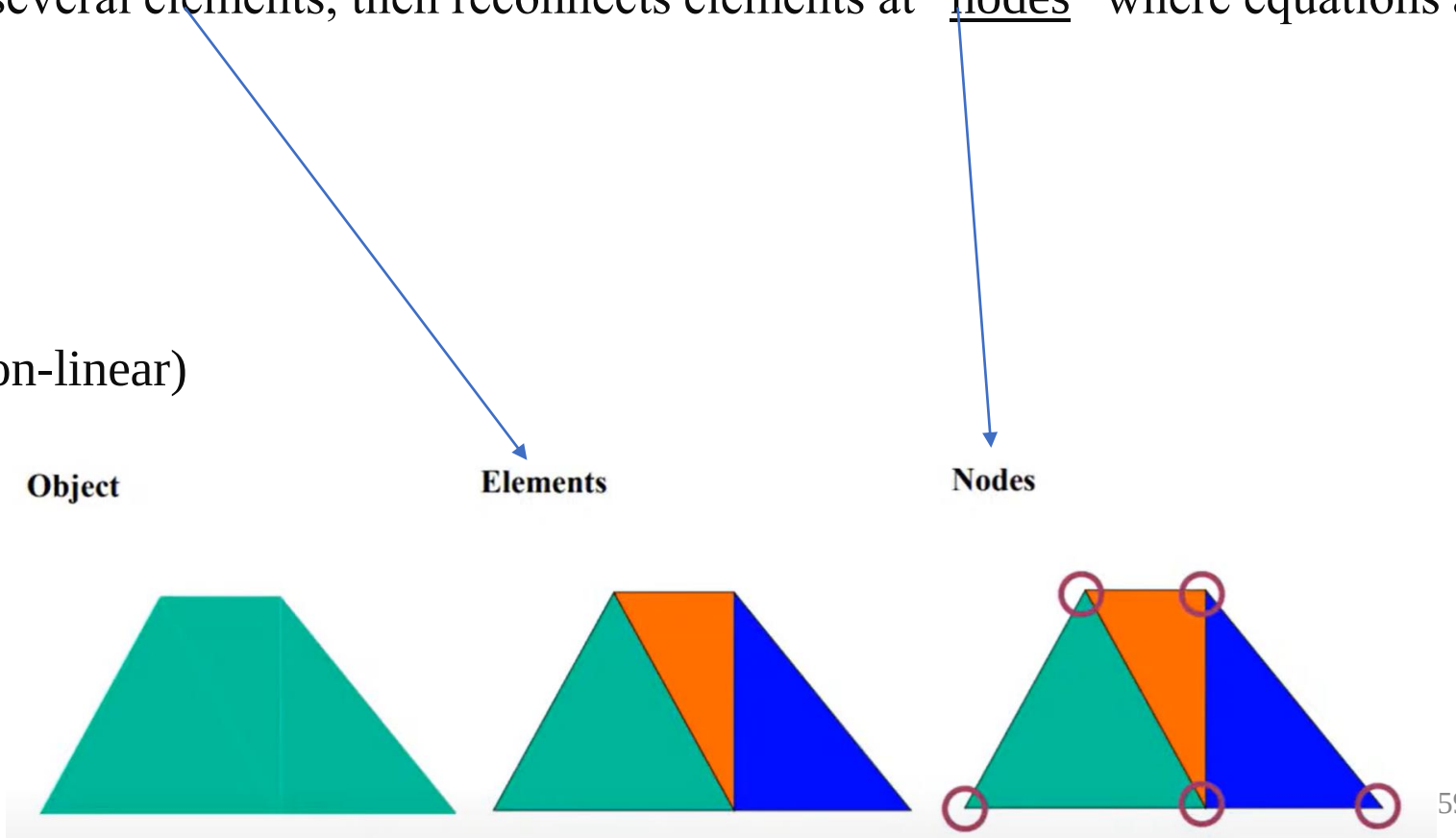
- Continuum: Infinite
- FEM: Finite (origin of the name FEM)
- FEM divides a structure into several elements (pieces of the structure)
- Then reconnects elements at "nodes" as if nodes were pins or drops of glue that hold elements together
- This process results in a set of simultaneous algebraic equations
- Finite Element Method (FEM) is a numerical technique for finding approximate solutions to boundary value problems for partial differential equations. It is used predominantly in engineering, especially for structural, thermal, and fluid analysis.
- The term FEM was first coined by Ray William Clough ("Legend of Earthquake Engineering") in 1960.
- Most commercial FEM packages (such as ANSYS, Adina, Abaqus) originated in 1970.

Foundations of FEM

- Engineering phenomenon can be expressed by governing equations and boundary conditions
- FEM approximates PBEs into a set of simultaneous algebraic equations:

  [K]{u} = {F}, where K are material properties, u is the behavior, F is the action applied;
- **Behavior *u* is unknown and should be solved/analyzed/plotted; $\{u\} = [K]^{-1}\{F\}$**
- FEM divides a structure into several elements, then reconnects elements at "nodes" where equations are solved
- **Applications:**
  - Mechanical/Aerospace
  - Civil/Automotive
  - Structural/Stress analysis

    (Static/Dynamic, Linear/Non-linear)
  - Fluid flow
  - Heat transfer
  - Electromagnetic fields
  - Soil mechanics
  - Acoustics
  - Biomechanics



Foundations of FEM

Analysis	Property [K]	Behavior {u}	Action {F}
Elastic	Stiffness	Displacement	Force
Thermal	Conductivity	Temperature	Heat source
Fluid	Viscosity	Velocity	Body force
Electrostatic	Permittivity	Electric potential	Charge

- Behavior *u* is unknown
- Knowing appropriate material properties is important; experimental/DFT/MD… data
- We will try to run one/a few examples of each of the above in the next module

$$[\mathbf{K}]\{\mathbf{u}\} = \{\mathbf{F}\} \quad \Rightarrow \quad \{\mathbf{u}\} = [\mathbf{K}]^{-1}\{\mathbf{F}\}$$

Property

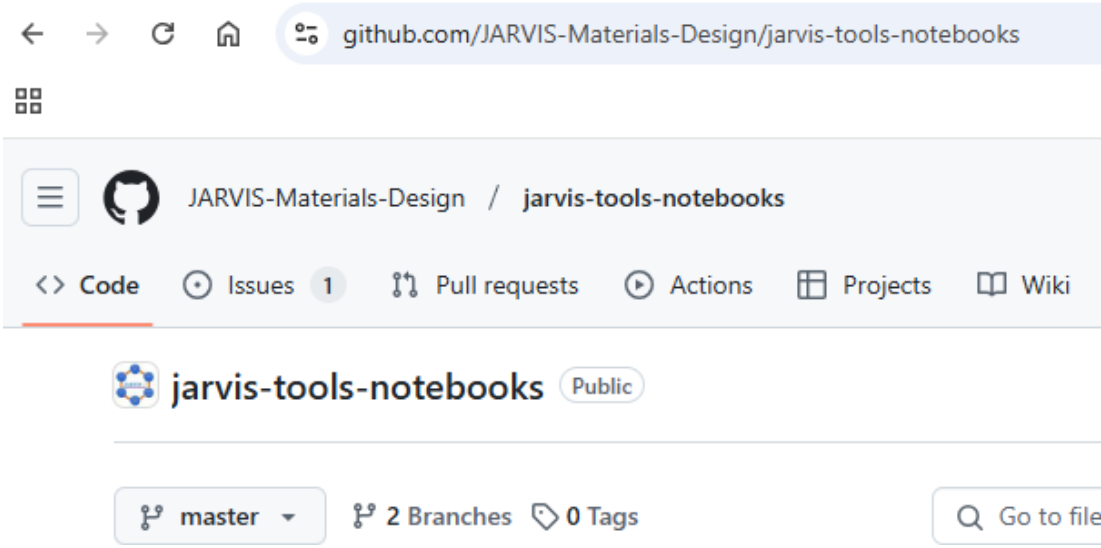
Behavior

Action

https://ocw.mit.edu/courses/16-810-engineering-design-and-rapid-prototyping-january-iap-2007/pages/lecture-notes/

Day 1 Hands-on Session

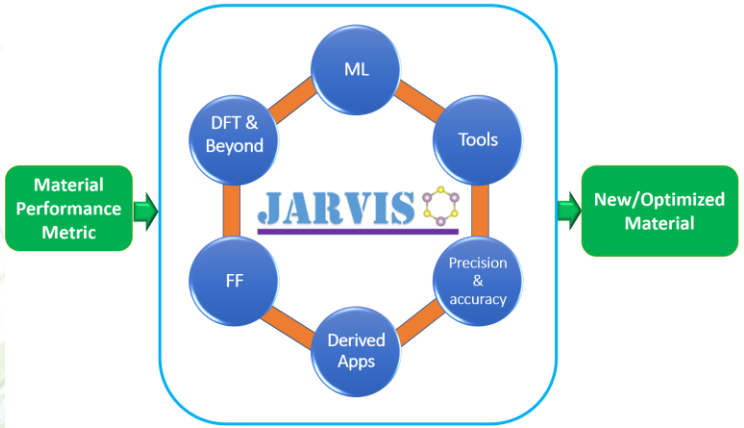
1. Go to website: https://jarvis.nist.gov/
2. Make an account, Go to one of the databases/interactive apps
3. On JARVIS website, click on Tutorials >> JARVIS-Tools-Notebooks link
4. B.1 HPC basics
5. B.2 Python beginners notebook
6. B.4 Silicon atomic structure and analysis example
7. ES. 1 Analyzing JARVIS-DFT data
8. ES.29 GPAW Colab
9. FF.1 JARVIS-LAMMPS



Materials Informatics: Fingerprints, Graph Neural Networks, and Transformers Based Models for Materials Design

Kamal Choudhary
Staff Scientist
NIST, Gaithersburg, MD, USA

Jan 20-25, 2025



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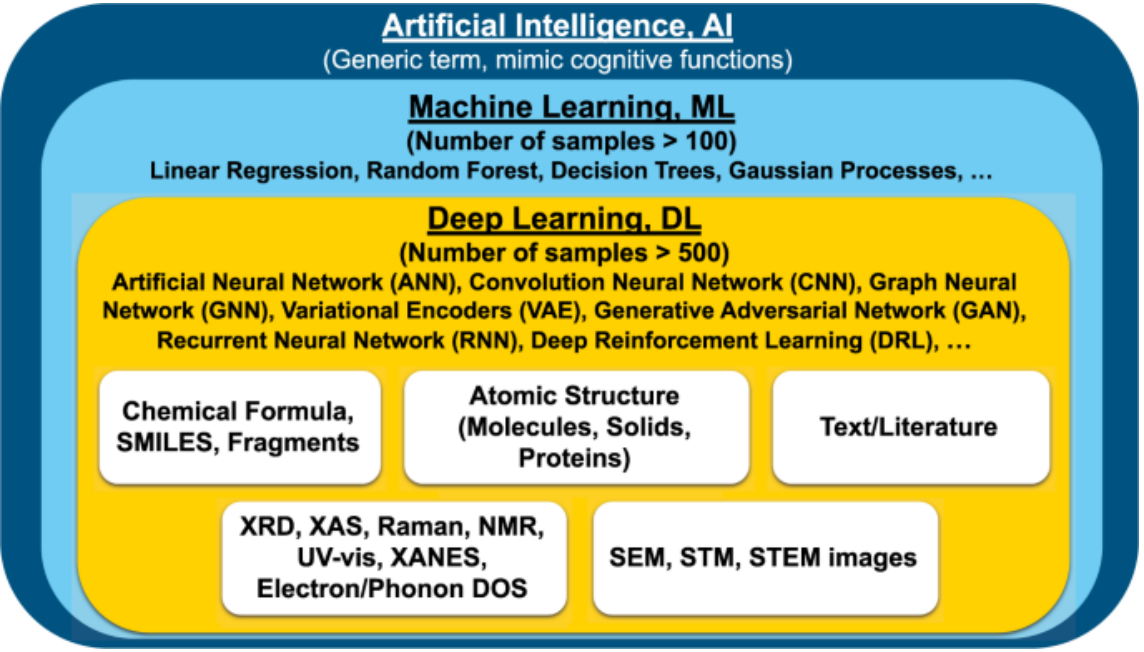
Day 3 Schedule

- Fundamentals of AI/ML
- Types of ML
- AI/ML ready Materials Databases
- Fingerprints/Descriptors, Conventional ML algorithms for Materials

What is AI/ML/DL?

- Artificial intelligence (AI) is a broad field of computer science that's concerned with building intelligent machines capable of performing tasks typically requiring human intelligence.
- Machine learning (ML) is a type of artificial intelligence (AI) that allows computers to learn without being explicitly programmed.
- Machines don't really know Materials/Mechanical Engineering etc., they deal with/know numbers.
- If multi-scale models guide experiments, ML methods can guide multi-scale modeling methods



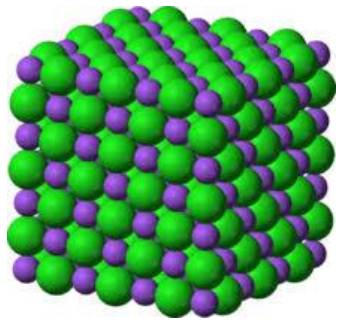
https://www.nature.com/articles/s41524-022-00734-6
https://www.deeplearningbook.org/

Motivation

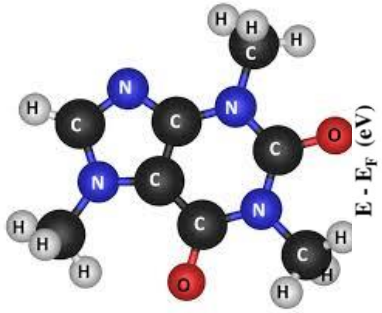
- **Multi-scale, multi-fidelity methods:**
  - **DFT/BeyondDFT,**
  - **FF,**
  - **AI,**
  - **Meso-scale,**
  - **Experiments**
- **Challenges with various data modalities:**
  - **Scalar,**
  - **Spectra,**
  - **Image,**
  - **Text etc.,**

Materials Genome Initiative 2011, $400 million

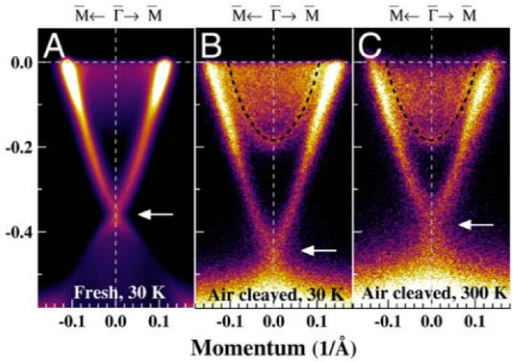
US CHIPS Act 2022, $52 billion



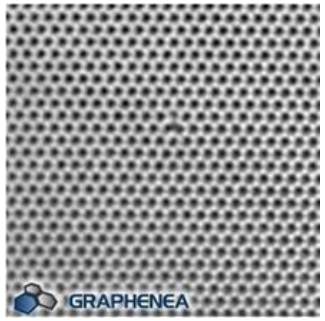
Crystals



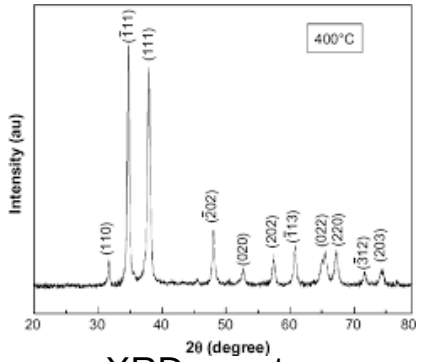
Molecules



Band-structure

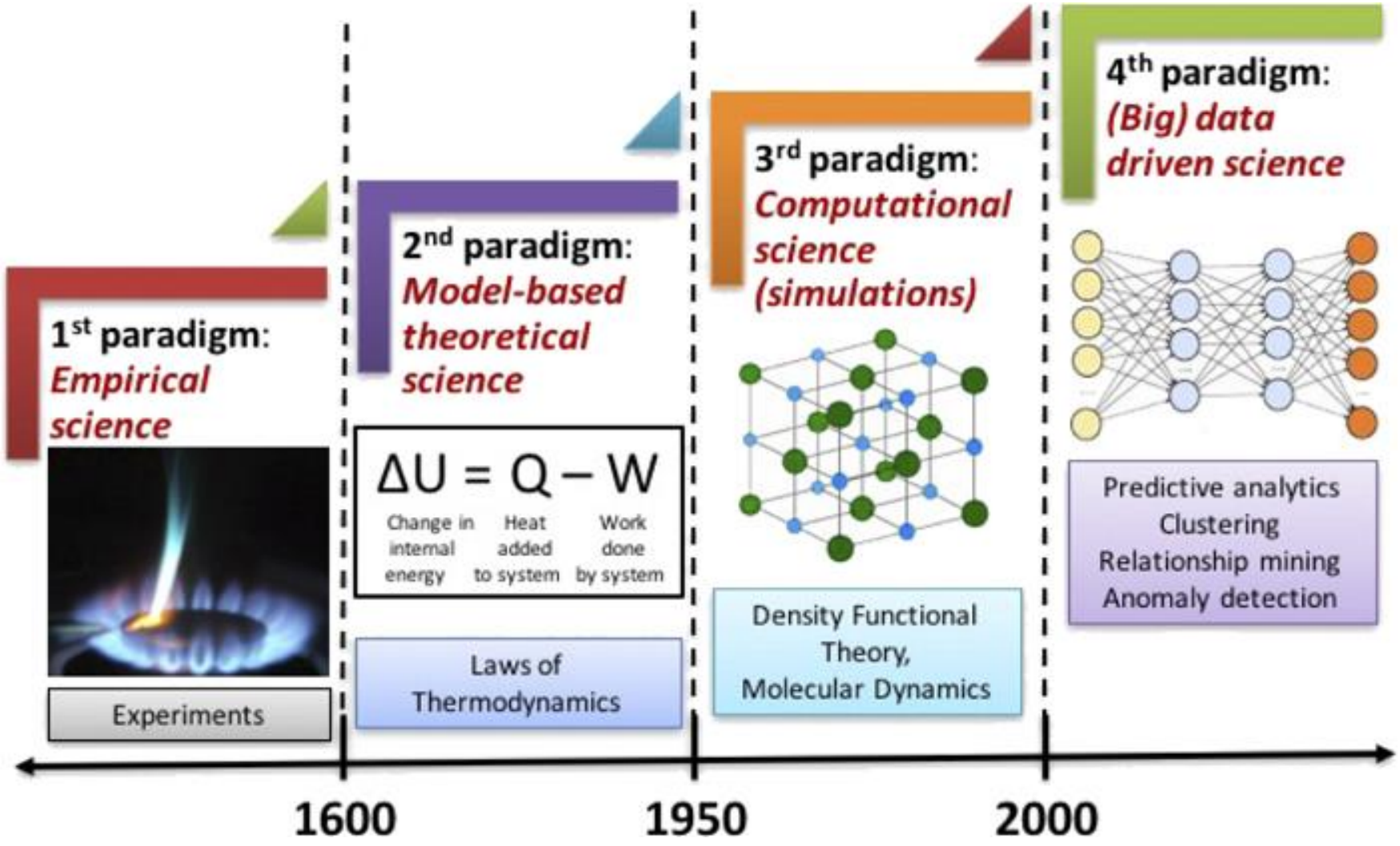


TEM images



XRD spectra

AI/ML as a Fourth Paradigm



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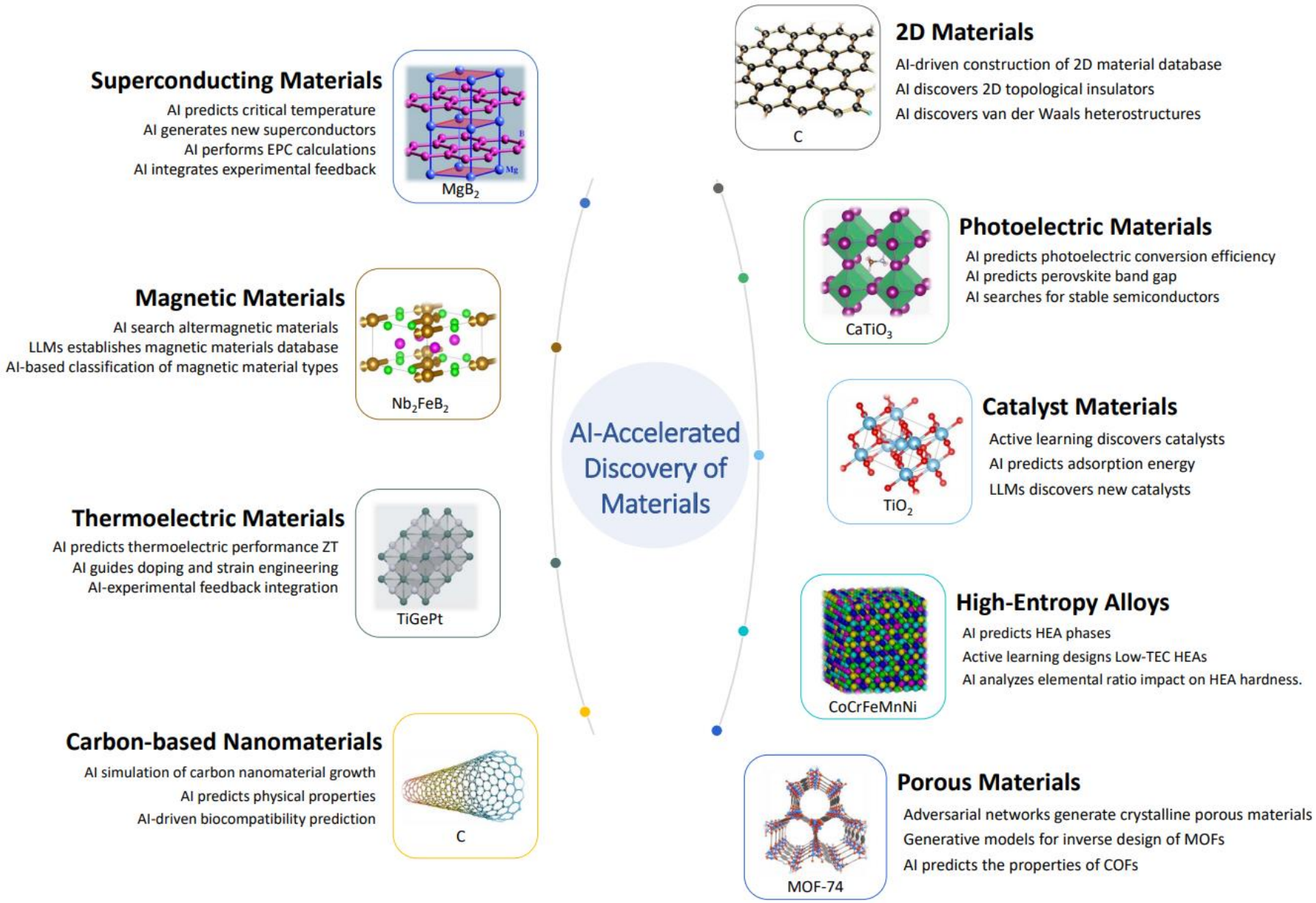
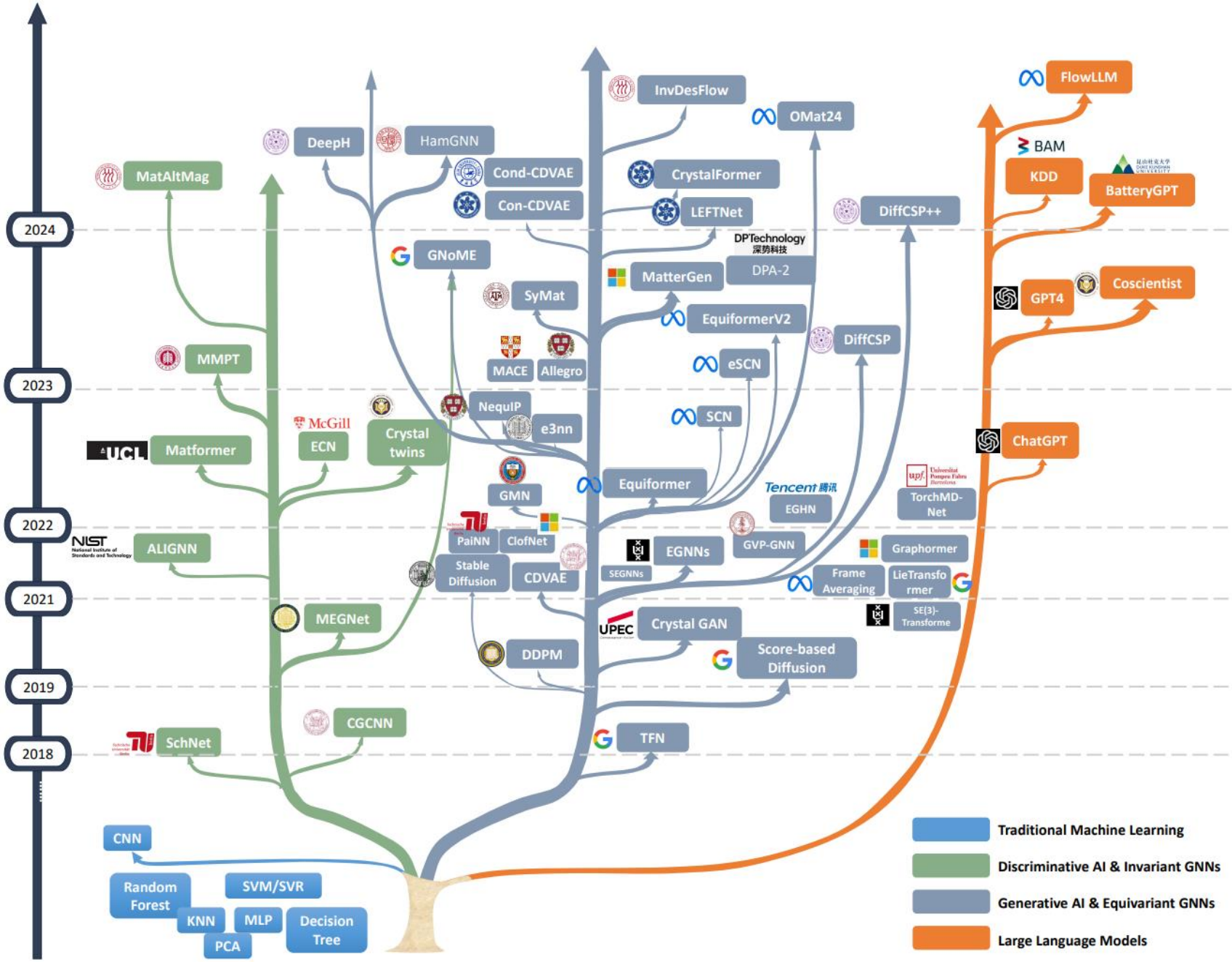
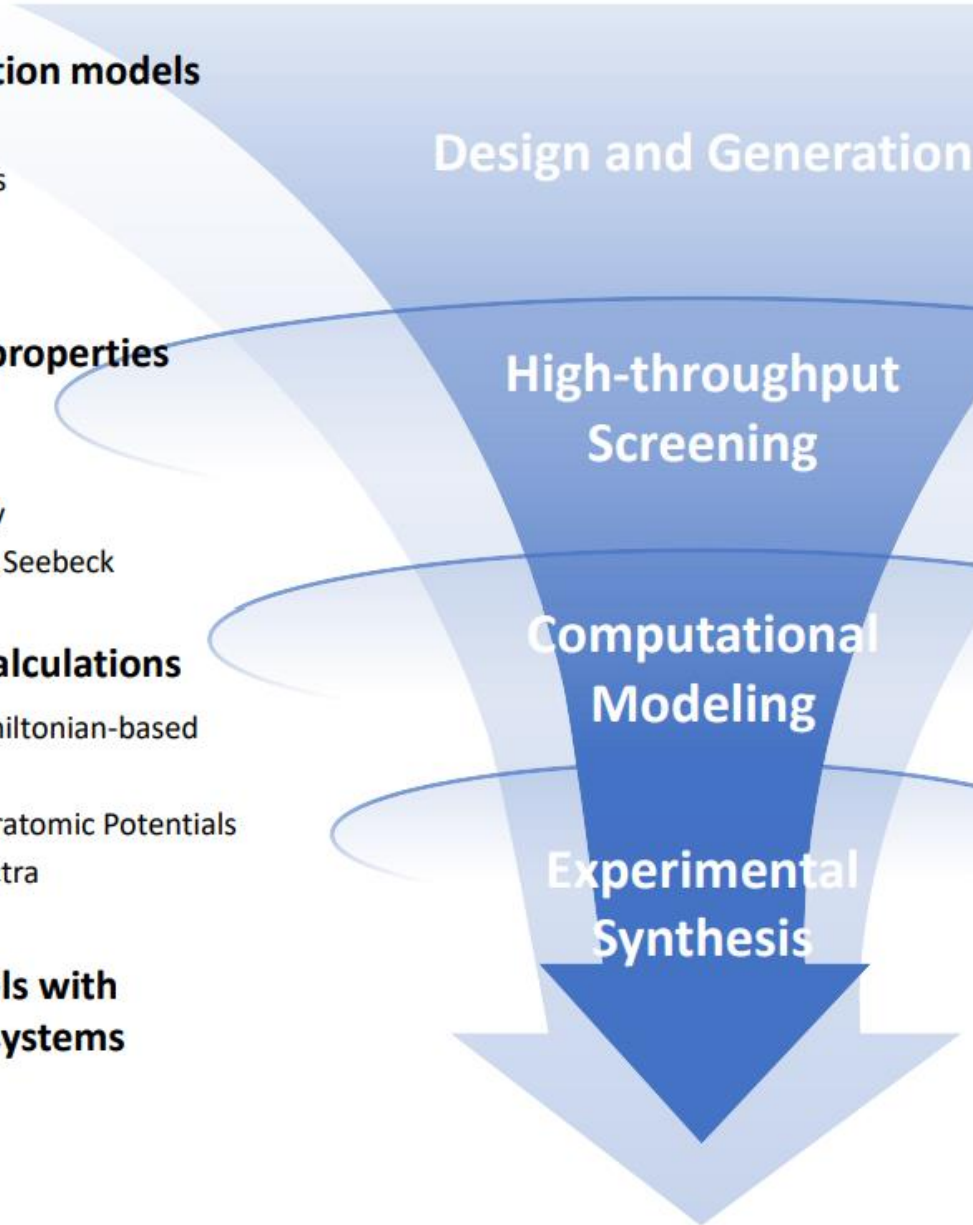


https://arxiv.org/pdf/2411.09429



https://arxiv.org/pdf/2411.09429

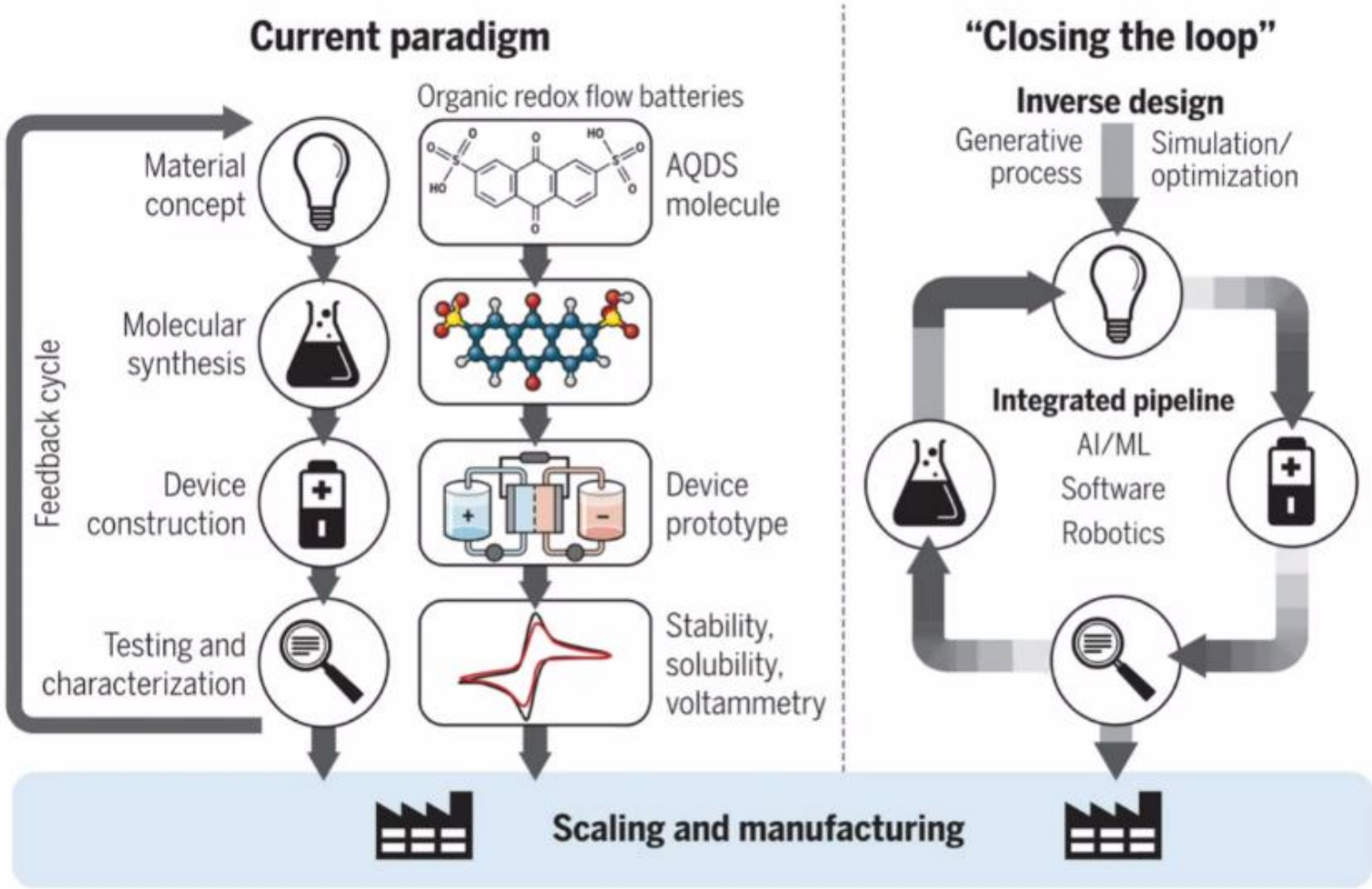


- **Conditional generation models**
  - Functional materials
  - Space group numbers
  - Heterostructure
  - Amorphous
- **AI predict material properties**
  - Formation energy
  - Band gap， Dos
  - Tc， superconductivity
  - Thermal conductivity, Seebeck coefficient, ZT value
- **AI-accelerated DFT calculations**
  - ML techniques for Hamiltonian-based Ab Initio Calculations
  - Machine Learning Interatomic Potentials
  - AI predict phonon spectra
  - AI predict EPC
- **Integrating ML models with robotic automation systems**

- **Benchmarks， Dataset**
- **Chemical composition generation**
- **LLMs generation**
- **AI structural relaxation**
- **Active Learning screening**
- **LLMs ranking**
- **Deep-learning DFT Hamiltonian**
- **Density Functional Perturbation Theory**
- **Dynamic adjustment of predictive models with real-time experimental data**

https://arxiv.org/pdf/2411.09429

CLOSING THE LOOP WITH SELF-DRIVING LABS



Sánchez-Lengeling and Aspuru-Guzik, **Science**, 361, 360, (2018).

Types of ML

- **Supervised Learning**:
  - Involves training a model on a labeled dataset, where the desired output is known.
  - Common algorithms: Linear Regression, Support Vector Machines (SVM), Neural Networks.
  - Example: Predicting material strength based on composition/structure and processing conditions.
  - Types:
    - Classification: categorical output (e.g. cat vs dog classification of images)
    - Regression: continuous output (e.g. weight of a cat)

- **Unsupervised Learning**:
  - Involves training a model on an unlabeled dataset, where the desired output is unknown.
  - Common algorithms: K-means Clustering, Principal Component Analysis (PCA).
  - Example: Identifying patterns in manufacturing defects without prior knowledge of defect types.

- **Reinforcement Learning**:
  - Involves training a model to make a sequence of decisions by rewarding desirable actions.
  - Common algorithms: Q-learning, Deep Q-Networks (DQN).
  - Example: Optimizing the control parameters of a robotic arm in real-time.

Applications of ML in Materials Engineering

- **Material Property Prediction**:
  - Use ML models to predict properties such as yield strength, elasticity, and thermal conductivity.
  - Example: Using neural networks to predict the stress-strain behavior of novel alloys.

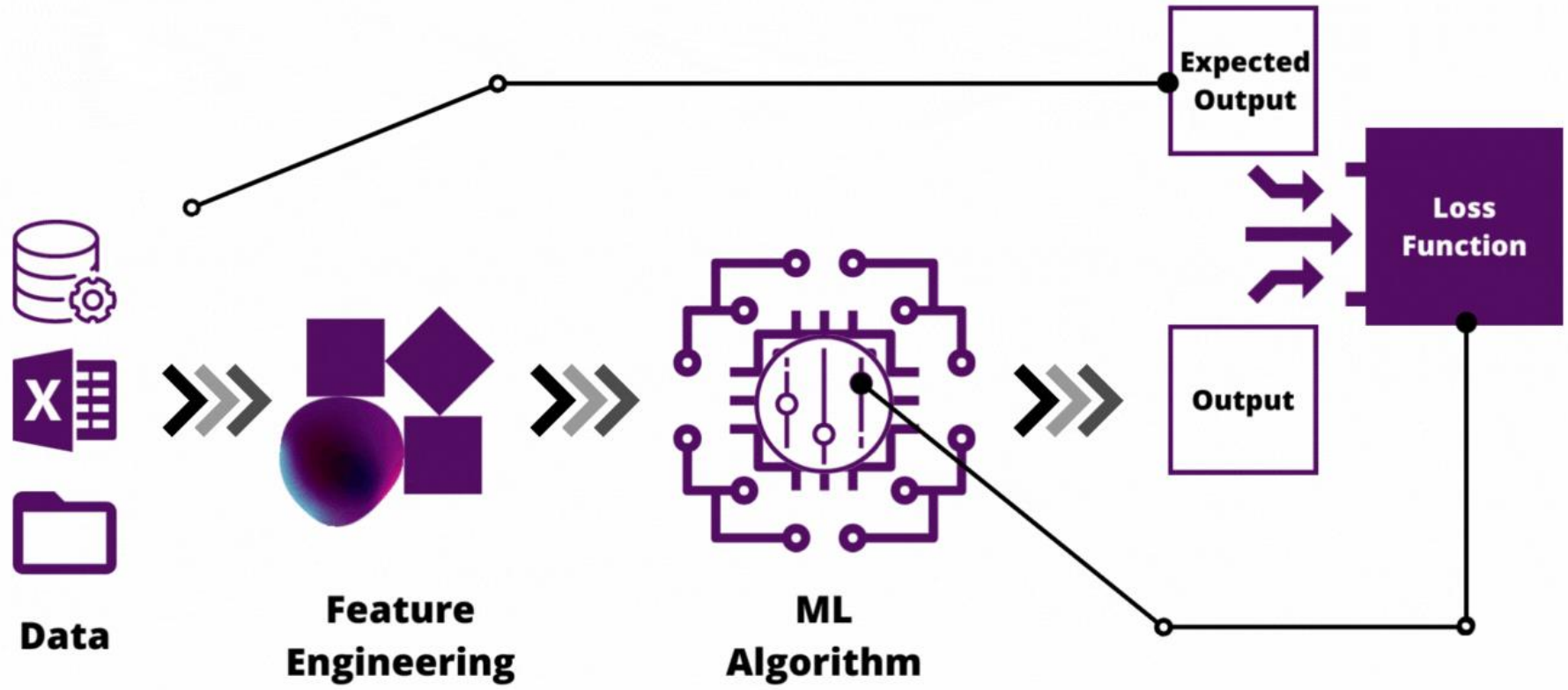
- **Design Optimization**:
  - Apply ML algorithms to optimize design parameters for mechanical components.
  - Example: Using genetic algorithms to optimize the shape of an airfoil for maximum lift-to-drag ratio.

- **Fault Detection and Diagnosis**:
  - Implement ML models to detect and diagnose faults in mechanical systems.
  - Example: Using SVM to classify different types of wear in bearings based on vibration data.

- **Predictive Maintenance**:
  - Utilize ML for predictive maintenance by analyzing historical data to predict future failures.
  - Example: Using time-series analysis to predict the remaining useful life of machinery.

- **Process Control and Automation**:
  - Develop intelligent control systems using reinforcement learning.
  - Example: Optimizing the welding process parameters in real-time to ensure consistent quality.

General Procedure of ML



1. Data (Define problem, Data collection & Visualize)
2. Model selection
3. Training
4. Evaluation & Deployment

Define the problem

Determine objective: Clearly define the problem you want to solve and the goals you want to achieve with machine learning.

- **Understand the Problem**: Identify the specific issue or opportunity that machine learning can address.
- **Define Objectives**: Set clear, measurable objectives for the project (e.g., improve prediction accuracy, reduce operational costs).
- **Scope the Project**: Determine the scope, including the data to be used, the timeline, and the resources required.

Determine type of task:

- Supervised,
- Unsupervised,
- Reinforcement learning,
- A combination?

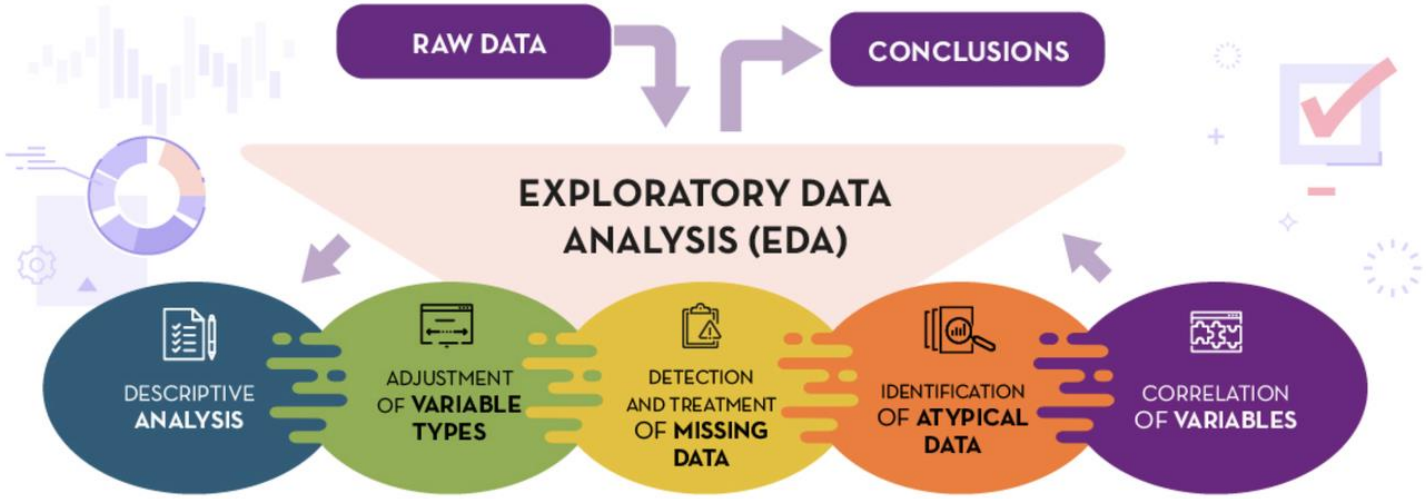
Source: pinterest

Data collection

- **Objective**: Gather the data needed to train and evaluate the machine learning model, Garbage In, Garbage Out (GIGO).
- **Identify Data Sources**: Determine where the data will come from (e.g., sensors, databases, public datasets).
- **Collect Data**: Gather the data, ensuring it is relevant and sufficient for the problem at hand.
- **Data Storage**: Store the collected data in a structured format suitable for analysis.
  - Atomic structure (RCSB PDB, JARVIS-DFT, Materials Project, OQMD, AFLOW),
  - Coarse-grain: CGProt, MSCG , ENM-DB,
  - Phase field dataset: PFHub, CALPHAD-DB,
  - FigShare, Kaggle, Zenodo, GitHub & many more …

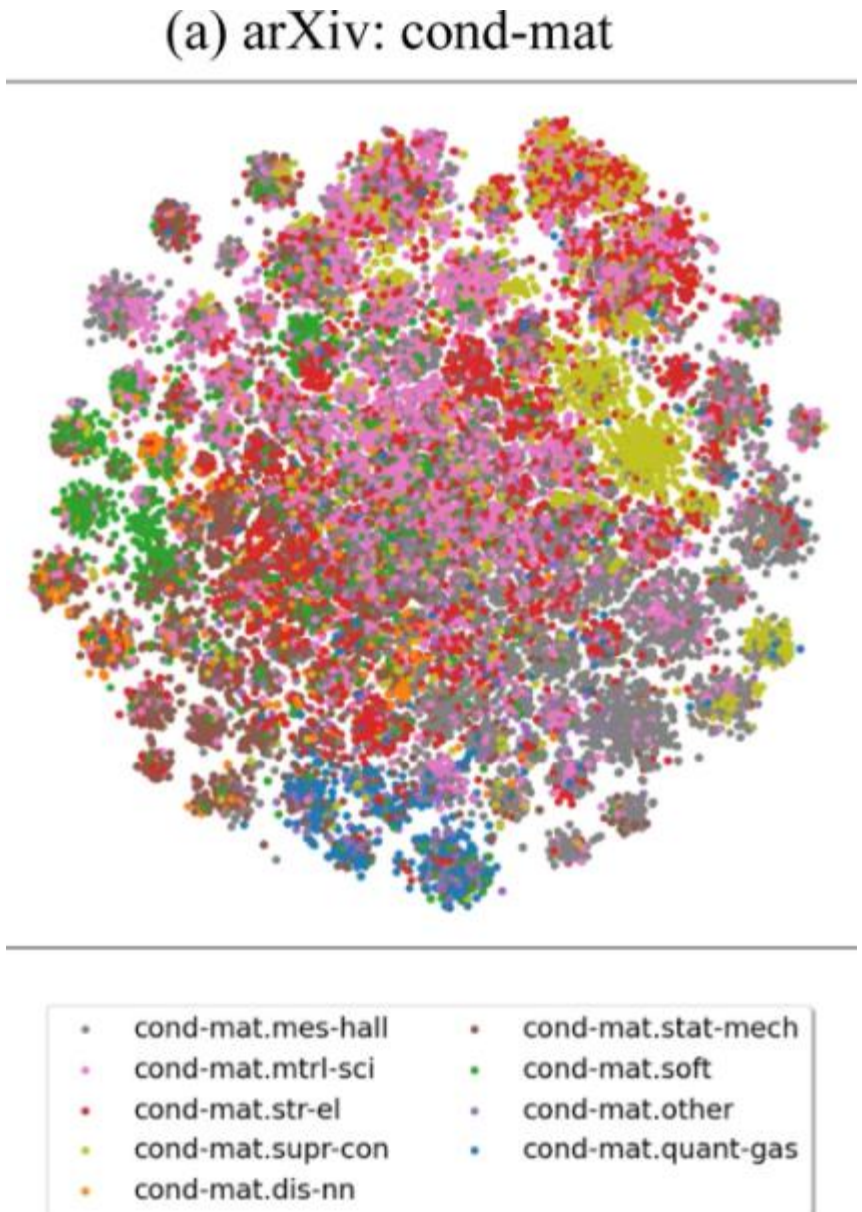
Exploratory Data Analysis (EDA)

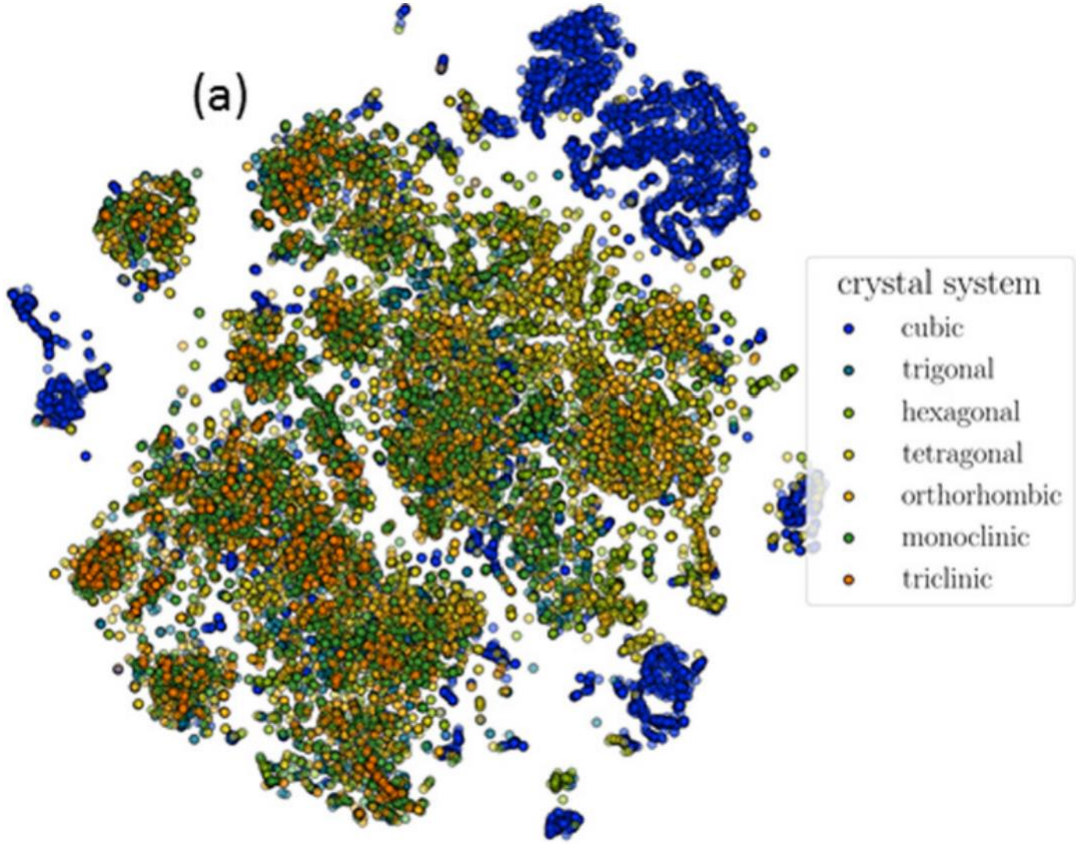
- **Descriptive Statistics**: Calculate summary statistics to understand the distribution and central tendencies of the data.
- **Data Visualization**: Use plots (e.g., histograms, scatter plots, box plots) to visualize data distributions and relationships.
- **Correlation Analysis**: Identify correlations between features to understand their relationships and potential multi-collinearity issues.



https://www.linkedin.com/pulse/exploratory-data-analysis-eda-unveiling-story-hidden-manish-rawat/

PCA/t-SNE/UMAP/Histograms

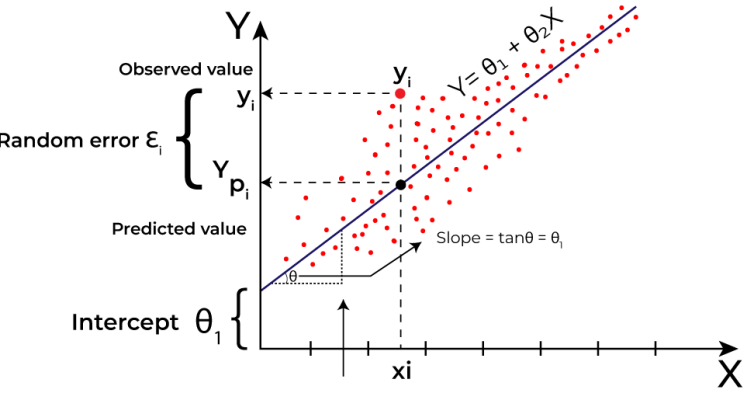




UMAP (Uniform Approximation and Projection)
t-SNE (t-distributed stochastic neighbor embedding)
PCA (Principal component analysis)
… (using Scikit-Learn package, CFID, ChemNLP)

ML Models

Linear Regression



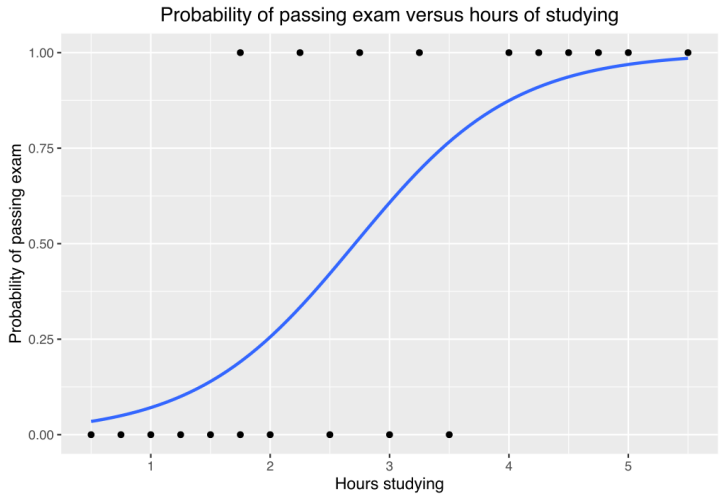
$$y = \beta_0 + \beta_1 x$$

- y is the dependent variable.
- x is the independent variable.
- β0 is the y-intercept of the line.
- β1 is the slope of the line.
- To estimate $\beta 0$ and $\beta 1$, we minimize the sum of the squared residuals:

$$\text{RSS} = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2$$

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p$$

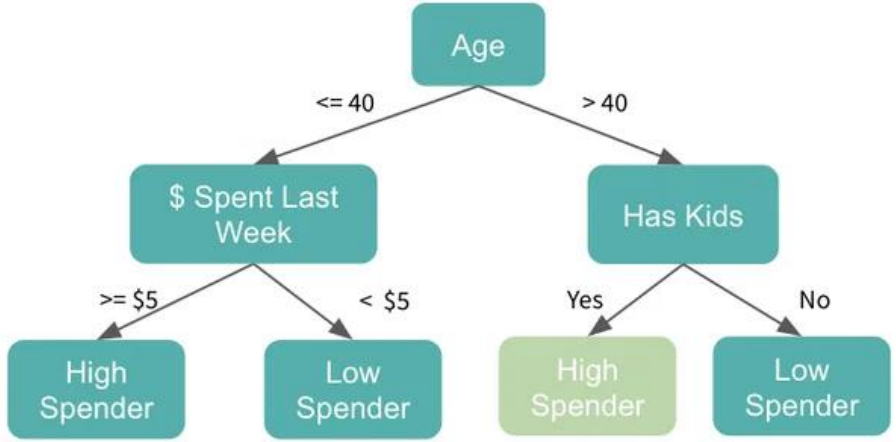
Logistic Regression



- Log-odds of an event as a linear combination of one or more independent variables
- Used for predicting a binary or categorical dependent variable.

$$p(x) = \frac{1}{1 + e^{-(x-\mu)/s}}$$

Tree based methods



Tree-based models use a series of if-then rules to generate predictions from one or more decision trees: RandomForest, GBM

Gini Impurity:

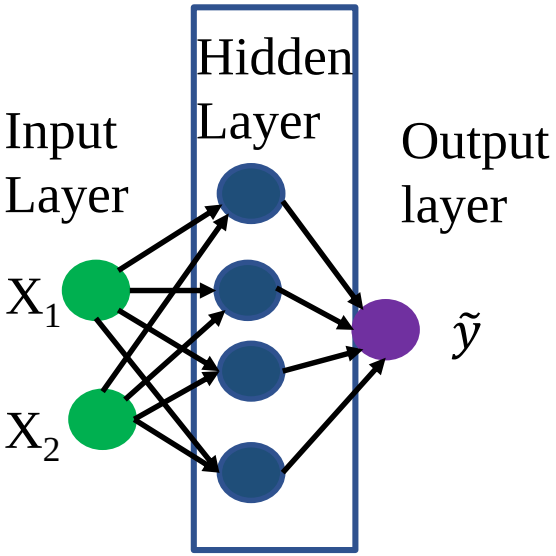
$$Gini = 1 - \sum_{i=1}^{n} p_i^2$$

Where p_i is the proportion of samples belonging to class i in the node.

$$Entropy = -\sum_{i=1}^{n} p_i \log_2(p_i)$$

ML Models

Standard NN



1) Forward propagation

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

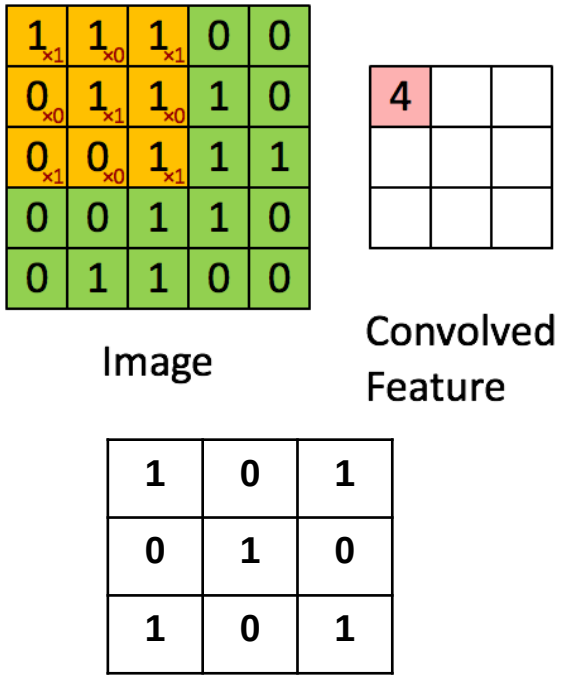
$a^{[1]} = \sigma(z^{[l]}); \quad a^{[0]} = X$

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

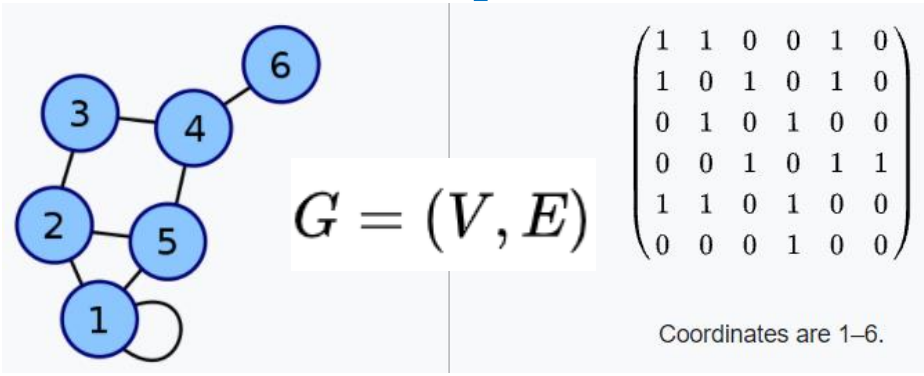
1) Convolution:
element-wise multiplication & sum

2) Pool: Max, Average, Sum

3) Fully Connected: Standard NN

Shared weights (Learnable filters), regularized version of NNs

GraphConvNN



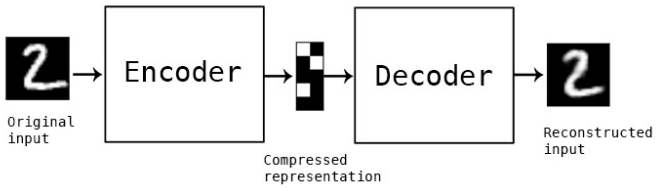
Types: un/weighted, un/directed, line, Hetero/Homogenous, Multigraph

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 <u>local</u>, neighborhood of a node only, independent of graph size

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

ML Models

AutoEncoders



Used for Dimensionality reduction or feature learning:

1) Encoding functions: *x* to a latent dimension *z*

$$\mathbf{z} = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$$

2) Decoding functions: *z* to x

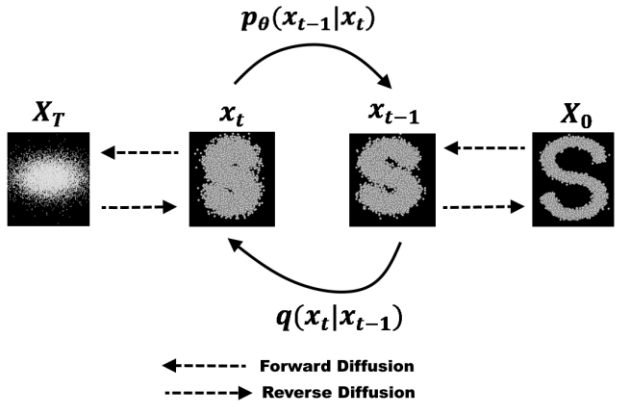
$$\mathbf{x}' = \sigma'(\mathbf{W}'\mathbf{z} + \mathbf{b}')$$

3) Loss function

$$\mathcal{L}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|^2$$

$$\|\mathbf{x} - \sigma'(\mathbf{W}'(\sigma(\mathbf{W}\mathbf{x} + \mathbf{b})) + \mathbf{b}')\|^2$$

Diffusion Models



Reverse diffusion process, starting from random noise

1)Forward diffusion: gradually adds noise over time steps

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) := \prod_{t=1}^{T} \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

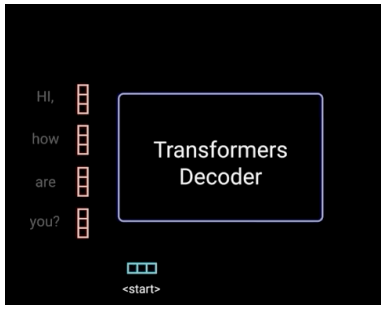
2) Reverse Diffusion Process:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) := \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

3) Training Objective and sampling:

$$L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}}[\, \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\|^2 \,]$$

Transformers



1) Self-attention: calculates the relevance between each pair of input tokens.

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

2) Multi-head attention: focus on different parts of the input sequence simultaneously

3) $\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W^O$

$$\text{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

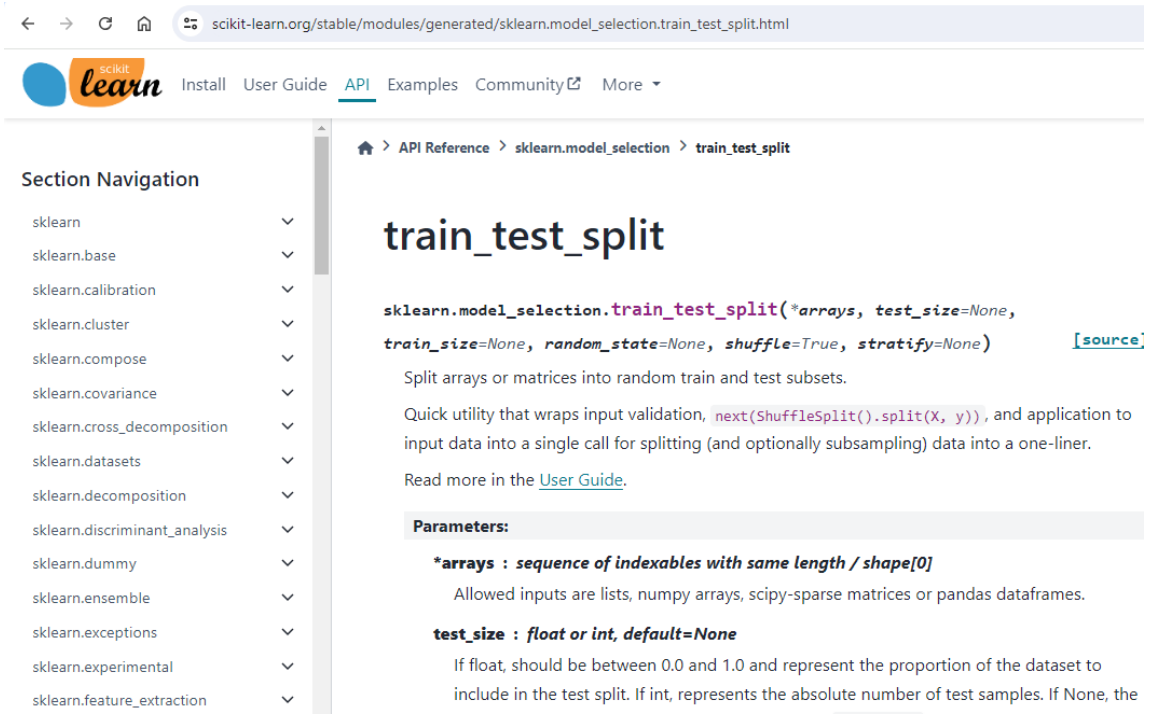
4) Positional Encoding: instead of RNN, use PE to convey the order of elements in the sequence

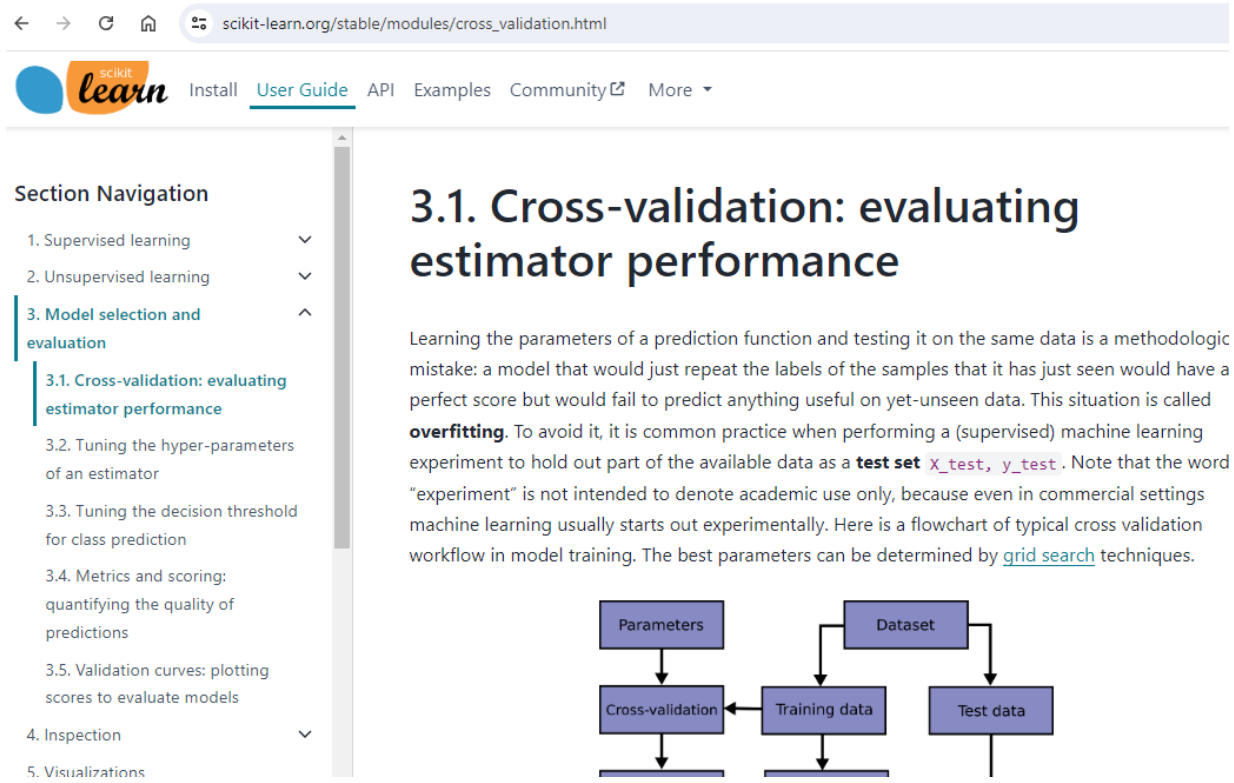
$$\text{PE}_{(pos,2i)} = \sin\left(\frac{pos}{10000^{2i/d_{\text{model}}}}\right)$$

$$\text{PE}_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{2i/d_{\text{model}}}}\right)$$

Model Training

- **Split Data**: Divide the data into training and testing (or validation) sets, because its hard to generate new data for testing models; usually 80 % training, 20 % testing data
- **Cross-validation**: Perform train-test split multiple times (say 5 or 10 times) to avoid data-split bias
- **Train Model**: Use the training set to train the model, adjusting parameters as needed.
- **Hyperparameter Tuning**: Optimize hyperparameters using techniques such as grid search or random search.





https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.train_test_split.html
https://scikit-learn.org/stable/modules/cross_validation.html

Objective/Loss Function Optimization & Gradient Descent

- Gradient descent is a fundamental optimization algorithm used for minimizing the cost function in machine learning and deep learning models.
- Types of GD:
  - Batch gradient descent: cost function is computed using the entire training dataset
  - Mini-batch gradient descent: computes the gradient using a small random subset (mini-batch) of the training data at each iteration
  - Stochastic (S)GD: the gradient of the cost function is computed using a single training example at each iteration
  - Gradient descent with Momentum: accumulates a velocity vector in directions of persistent reduction in the cost function and uses it to update the parameters
  - Adagrad (Adaptive Gradient Algorithm): adapts the learning rate for each parameter based on past gradients, making larger updates for infrequent parameters and smaller updates for frequent parameters
  - RMSprop (Root Mean Square Propagation): adaptive learning rate method that addresses Adagrad's diminishing learning rate issue
  - Adam (Adaptive Moment Estimation): Adam combines the ideas of momentum and RMSprop by maintaining a moving average of both the gradient and its square

Model Evaluation

- **Performance Metrics**: Evaluate the model using appropriate metrics:
  - Classification: accuracy, precision, recall, F1-score
  - Regression: R^2, mean absolute error, root mean squared error.
- **Baseline/Random guessing model**:
  - For classification (1/N; N: number of classes),
  - For Regression: take average of training samples and use it as predictions for the test set (average guessing model); MAD/MAE should be > 1
- **Cross-Validation**: Use cross-validation to ensure the model generalizes well to unseen data.
- **Compare/Benchmark Results**: Compare the performance of the model to baseline models or previous iterations.

$$\text{Accuracy} = \frac{\text{Number of correct predictions}}{\text{Total number of predictions}}$$

$$R = \frac{\sum_{i=1}^{N}\left(y_i - \bar{y}\right)\left(\widehat{y_i} - \bar{\hat{y}}\right)}{\sqrt{\sum_{i=1}^{N}\left(y_i - \bar{y}\right)^2 \sum_{i=1}^{N}\left(\widehat{y_i} - \bar{\hat{y}}\right)^2}}$$

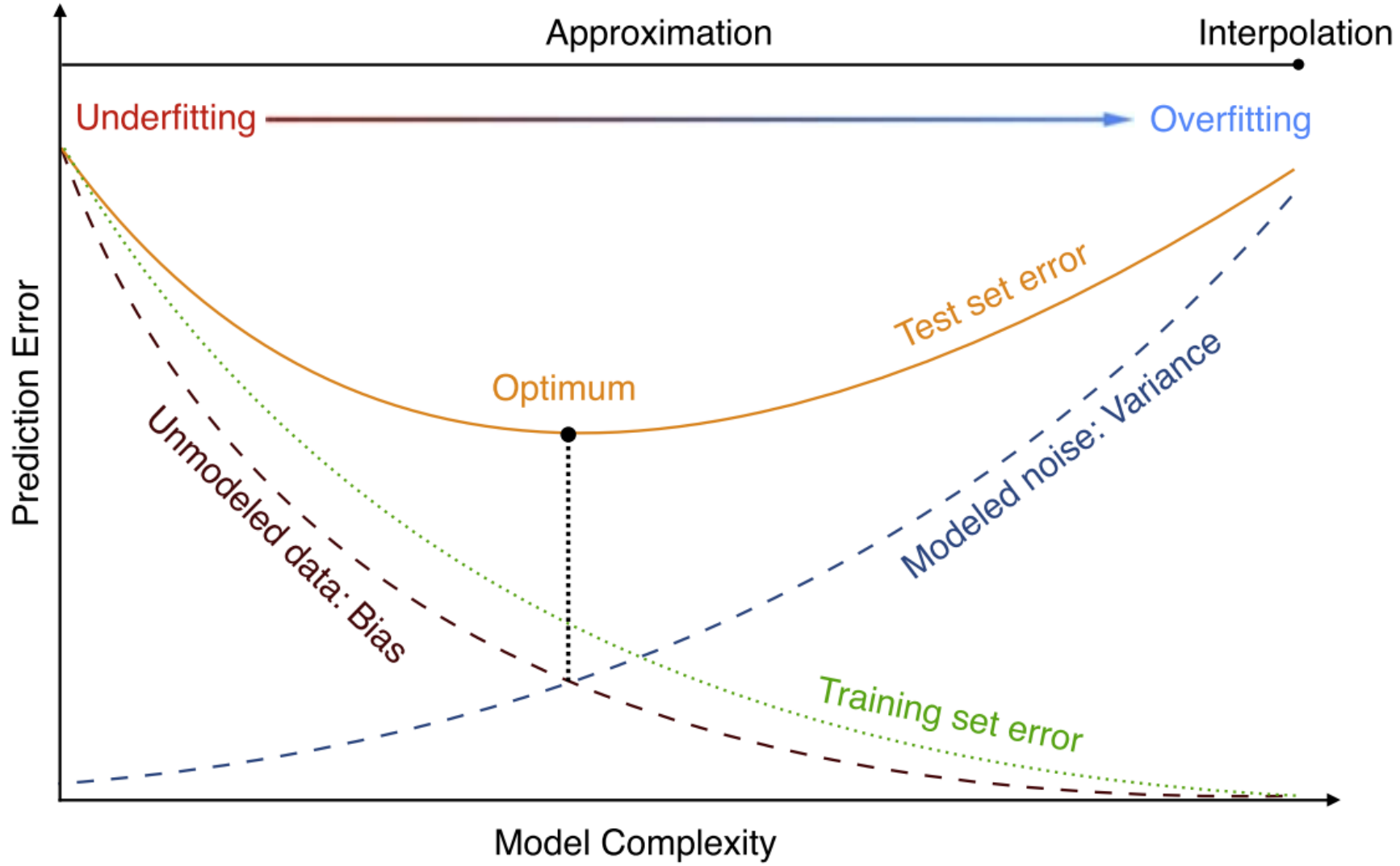
$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Where *TP* = True Positives, *TN* = True Negatives, *FP* = False Positives, and *FN* = False Negatives.

$$MAE = \bar{e} = \frac{1}{N}\sum_{N}\left|y - \hat{y}\right|$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{N}(y - \hat{y})^2}$$

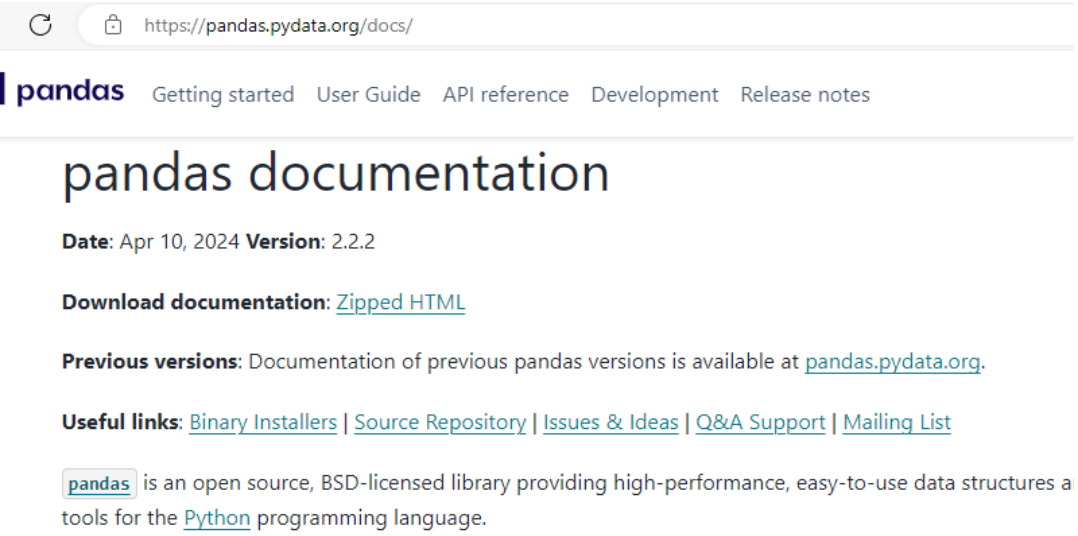
Bias Variance Trade off

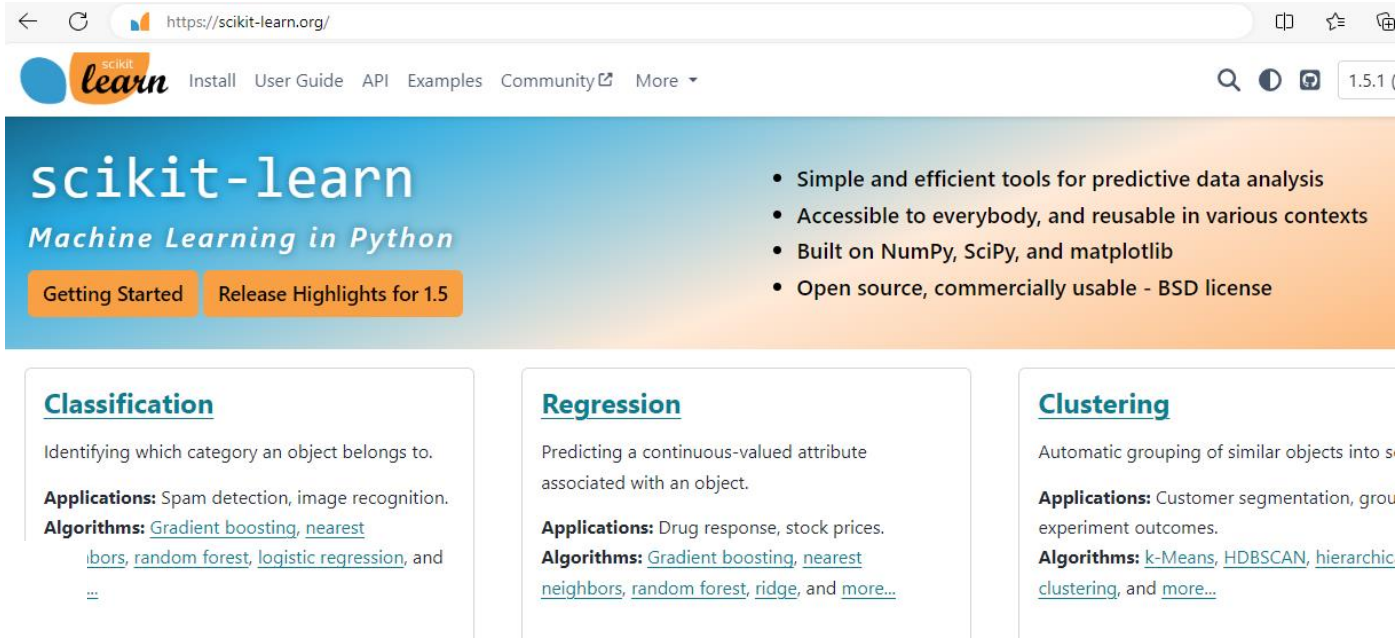


Model Deployment (for developers)

- **Deployment Options**: Choose how to deploy the model (e.g., as a web service, embedded in an application).
  - Flask, Django, Fast-API, StreamLit: e.g. Instagram developed with Django
  - Cloud based hosting: Amazon Web Services, Azure, Google Cloud
- **Integration**: Integrate the model with existing systems and workflows.
  - CI/CD (continuous integration/continuous development)
  - PyTest, CodeCoverage for checking code health everytime you make a change
- **Monitoring**: Set up monitoring to track the model's performance and detect any issues.
  - CRON job: automatically test every minute/hour/day/month

Software Libraries





Other Libraries:

- PyTorch, TensorFlow, JAX,
- Scikit-Image, OpenCV, Pillow,
- HuggingFace, JARVIS-Leaderboard etc.

AI/ML Review Articles/Books

JPhys Materials

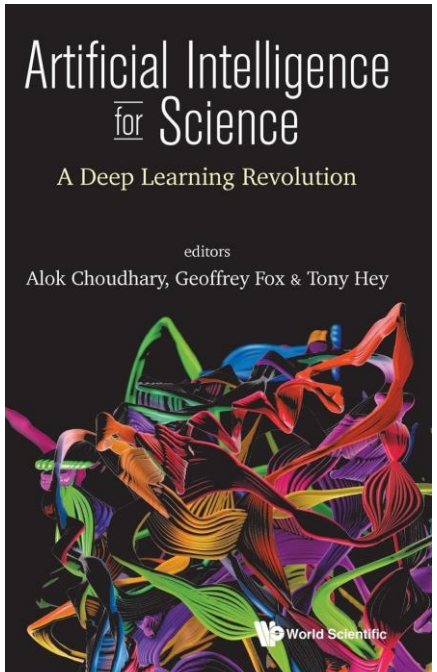
TOPICAL REVIEW

From DFT to machine learning: recent approaches to materials science–a review

Gabriel R Schleder[1,2,3], **Antonio C M Padilha**[2], **Carlos Mera Acosta**[1,2], **Marcio Costa**[2] and **Adalberto Fazzio**[1,2,3]

[1] Center for Natural and Human Sciences, Federal University of ABC, 09210-580, Santo André, São Paulo, Brazil
[2] Brazilian Nanotechnology National Laboratory/CNPEM, 13083-970, Campinas, São Paulo, Brazil
[3] Authors to whom any correspondence should be addressed.

E-mail: gabriel.schleder@ufabc.edu.br and adalberto.fazzio@lnnano.cnpem.br



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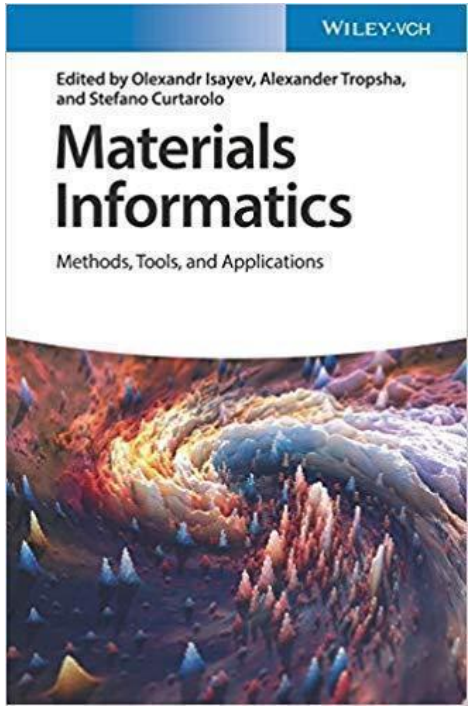
Review Article | Open access | Published: 05 April 2022

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

89k Accesses | **437** Citations | **36** Altmetric | Metrics

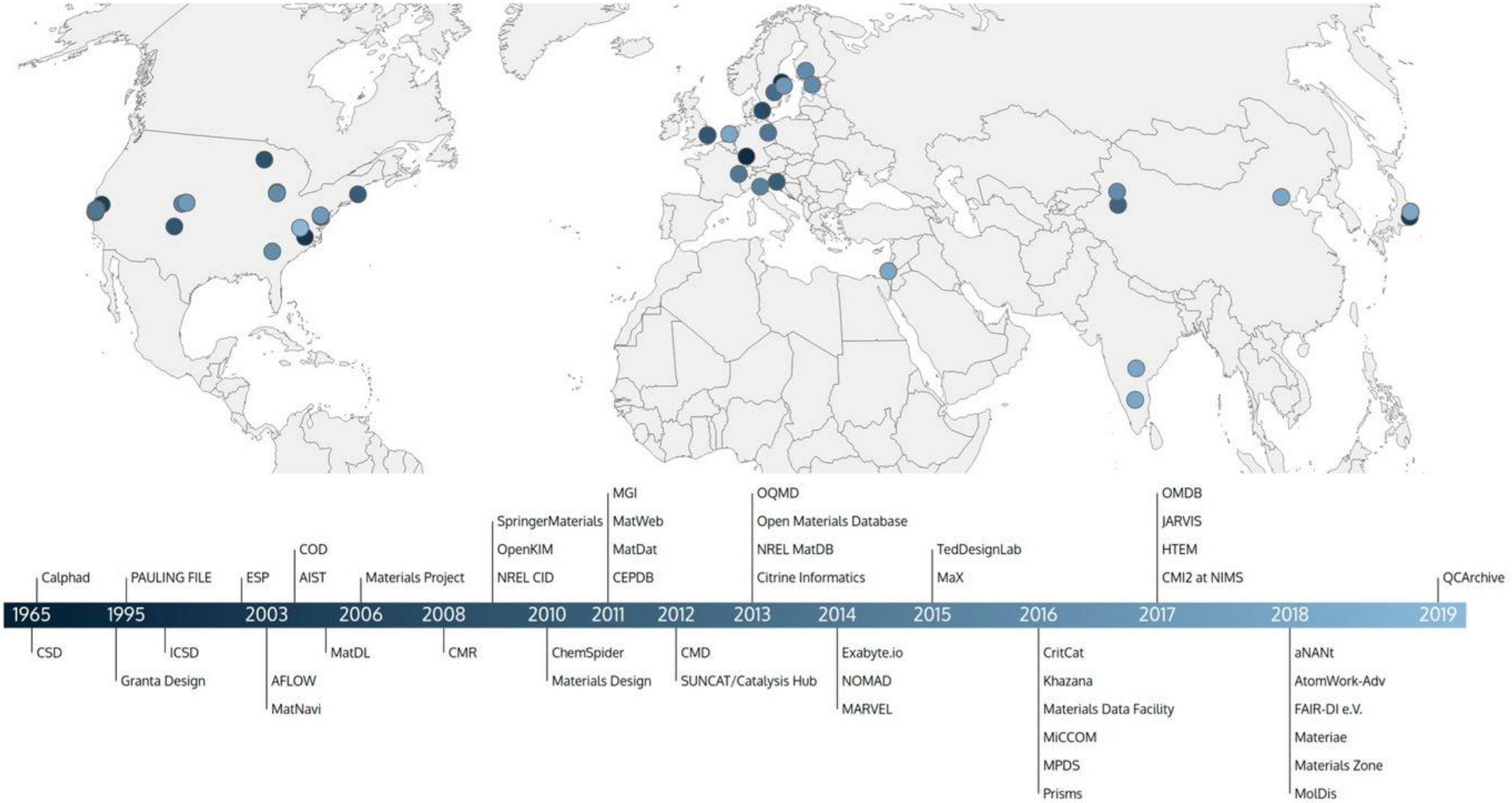


Databases

Table 1. Databases and software for DL atomistic design ('k', 'mil' = thousand, million).

Databases			
DB name	Datasize	Link	Ref.
JARVIS-DFT	56k	https://jarvis.nist.gov/jarvisdft/	3
JARVIS-FF	2.5k	https://jarvis.nist.gov/jarvisff/	3
MP	144k	https://materialsproject.org/	5
OQMD	816k	http://oqmd.org/	4
AFLOW	3.5mil	http://www.aflowlib.org/	6
QM9	134k	http://quantum-machine.org/datasets/	7
ANI	20mil	https://github.com/isayev/ANI1_dataset	96
MD17	1mil	http://quantum-machine.org/datasets	308
Tox21	760k	https://tox21.gov/resources/	309
CCCBDB	2069	https://cccbdb.nist.gov/	310
HOPV15	350	https://doi.org/10.6084/m9.figshare.1610063	311
C2DB	4000	https://cmr.fysik.dtu.dk/c2db/c2db.html	312
FreeSolv	504	https://github.com/MobleyLab/FreeSolv	313
NOMAD	11mil	https://nomad-lab.eu/prod/rae/gui/search	8
OPTIMADE	18mil	http://www.optimade.org/providers-dashboard/	314
Open catalyst project	1.2mil	https://opencatalystproject.org	315
MatBench	200k	https://matbench.materialsproject.org/	316
MCloud	22mil	https://www.materialscloud.org/home#statistics	317
CoreMOF	163k	https://mof.tech.northwestern.edu/	318
QMOF	22k	https://github.com/arosen93/QMOF	124
PDB	183k	https://www.rcsb.org/	319
PDBBind	23k	http://www.pdbbind.org.cn/	9
MOAD	39k	http://www.bindingmoad.org/	320

Databases



https://doi.org/10.1002/advs.201900808

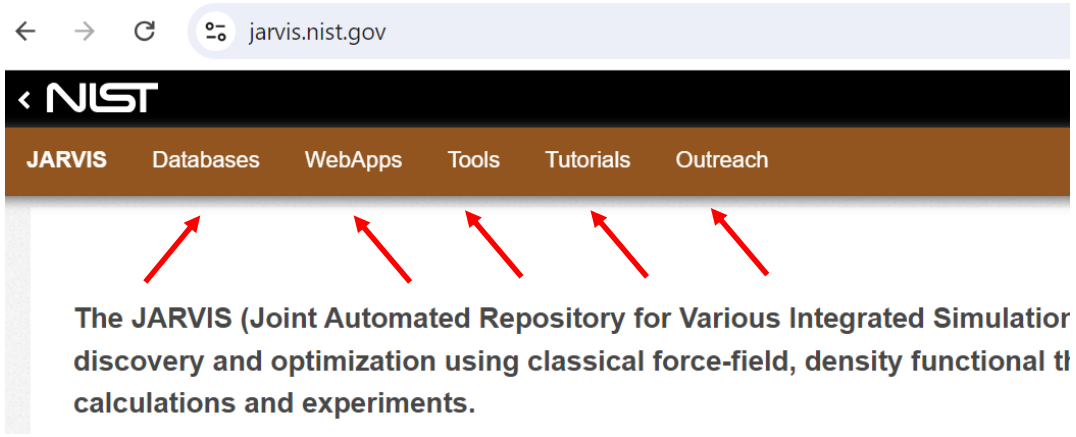
Software

Software packages			
Model name Ref.		Applications	Link
ALIGNN	Mol, Sol	https://github.com/usnistgov/alignn	65
SchNetPack	Mol, Sol	https://github.com/atomistic-machine-learning	69
CGCNN	Sol	https://github.com/txie-93/cgcnn	67
MEGNet	Mol, Sol	https://github.com/materialsvirtuallab/megnet	33
DimeNet	Mol	https://github.com/klicperajo/dimenet	68
MPNN	Mol	https://github.com/priba/nmp_qc	108
MatDeepLearn	Sol	https://github.com/vxfung/MatDeepLearn	321
GATGCNN	Sol	https://github.com/superlouis/GATGNN	322
ANI	Mol	https://github.com/isayev/ASE_ANI	96
Amp	Sol	https://bitbucket.org/andrewpeterson/amp	323
TensorMol	Mol	https://github.com/jparkhill/TensorMol	324
TorchMD	Mol	https://github.com/torchmd/torchmd	325
PROPhet	Sol	https://github.com/biklooost/PROPhet	326
DeepMD	Mol	https://github.com/deepmodeling/deepmd-kit	101,327
ænet	Sol	https://github.com/atomisticnet/aenet	328
E3NN	Mol	https://github.com/e3nn/e3nn	329
Neural			
fingerprint	Mol	https://github.com/HIPS/neural-fingerprint	330
DeepChemSt.	Mol	https://github.com/MingCPU/DeepChemStable	331
MoleculeNet	Mol, Sol	https://github.com/deepchem/deepchem	332
dgl-lifesci	Prot	https://github.com/awslabs/dgl-lifesci	66
gnina	Prot	https://github.com/gnina/gnina	110

Table 2. Software to apply DL to chemical formula, SMILES, and fragment representations.

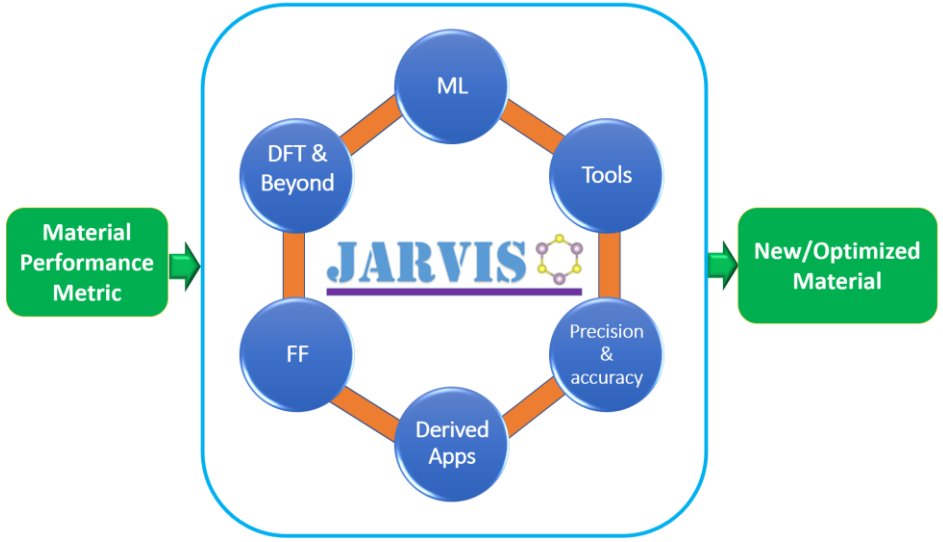
Chemical formula		
Model name	Link	Ref.
MatMiner	https://github.com/hackingmaterials/matminer	151
MagPie	https://bitbucket.org/wolverton/magpie	150
DScribe	https://github.com/SINGROUP/dscribe	158
ElemNet	https://github.com/NU-CUCIS/ElemNet	141
IRNet	https://github.com/NU-CUCIS/IRNet	152,153
Roost	https://github.com/CompRhys/roost	154
CrabNet	https://github.com/anthony-wang/CrabNet	333
CFID-Chem	https://github.com/usnistgov/jarvis/	90
Atom2vec	https://github.com/idocx/Atom2Vec	334
CrossPropertyTL	https://github.com/NU-CUCIS/CrossPropertyTL	157
SMILES and fragments		
DeepSMILES	https://github.com/baoilleach/deepsmiles	335
ChemicalVAE	https://github.com/aspuru-guzik-group/chemical_vae	336
CVAE	https://github.com/jaechanglim/CVAE	133
DeepChem	https://github.com/deepchem/deepchem	332
DeepFRAG	https://git.durrantlab.pitt.edu/jdurrant/deepfrag/	337
DeepFRAG-k	https://github.com/yaohangli/DeepFragK/	338
CheMixNet	https://github.com/NU-CUCIS/CheMixNet	339
SINet	https://github.com/NU-CUCIS/SINet	340

JARVIS-Database Overview



Collection of Databases, WebApps, Tools, Tutorials,…

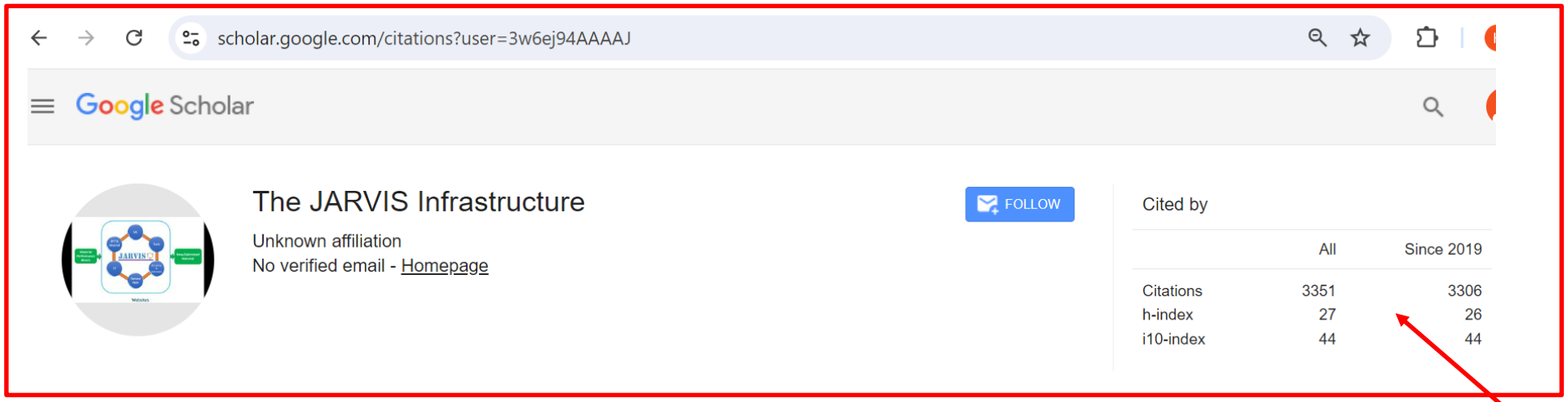
https://jarvis.nist.gov (Estd. 2017)

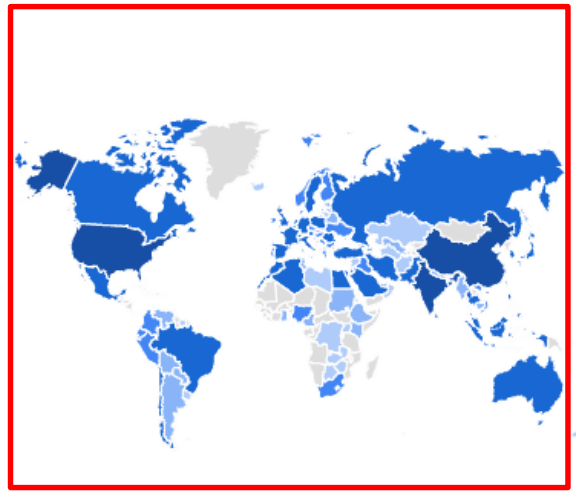


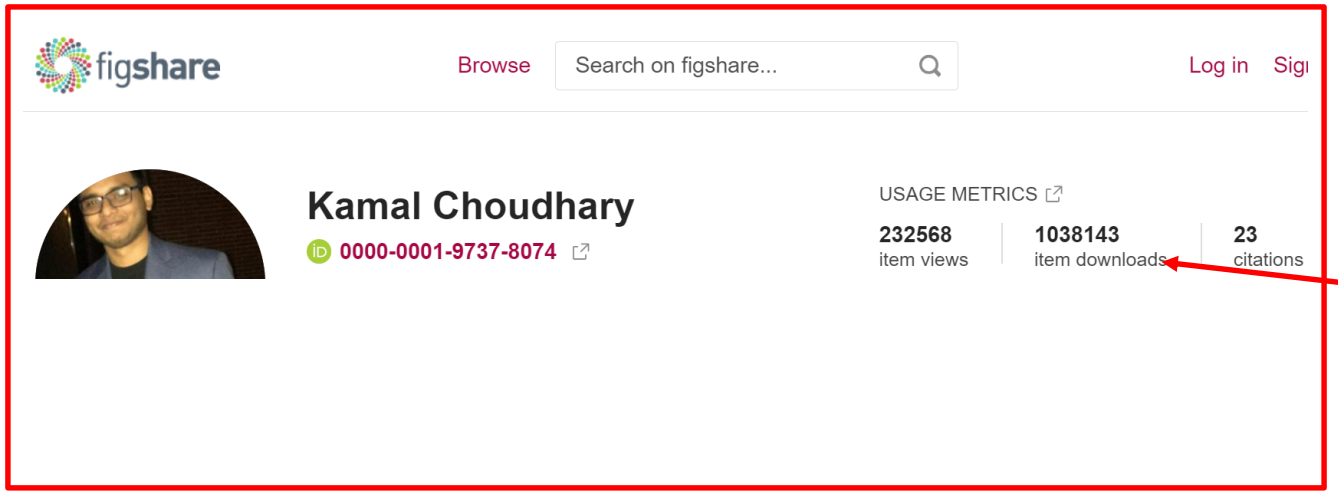
Materials Genome Initiative 2011, $400 million

US CHIPS Act 2022, $52 billion

Impact







Established: January 2017
Articles: 50+ articles, 3000+ citations
Users: ~200000 users worldwide
Materials: 80000+, millions of properties,
Downloads: ~1 M data download
~1 M code download

Choudhary et al., Nature: npj Computational Materials 6, 173 (2020)
Wines et al., Applied Physics Reviews 10 (4) (2023)

Databases

Name	Database/WebApp	Description
1. JARVIS-DFT	https://jarvis.nist.gov/jarvisdft	Density functional theory DB for 80000+ materials, >million properties
2. JARVIS-FF	https://jarvis.nist.gov/jarvisdft	Classical DB for ~2000 materials, >100 Classical FFs
3. JARVIS-CFID	https://jarvis.nist.gov/jarvisml	Classical force-field inspired (CFID) descriptors for conventional ML
4, ALIGNN, FF	https://github.com/usnistgov/alignn/	Atomistic Line Graph Neural Network for fast property prediction, unified FF for periodic table, structure optimization
5. AtomGPT	https://github.com/usnistgov/atomgpt	Atomistic Generative Pretrained transformer for forward and inverse materials design
6. InterMat & DefectMat	https://github.com/usnistgov/intermat & https://github.com/usnistgov/defectmat	Interface & Defect Materials Design Toolkit with DFT and AI methods
7. ChemNLP	https://github.com/usnistgov/chemnlp	Natural language processing for materials chemistry for arXiv/pubchem data
8. DAC	https://jarvis.nist.gov/jdac	Direct air capture/CO2 capture with AI trained on GCMC data
9. Leaderboard	pages.nist.gov/jarvis_leaderboard	Large scale benchmark platform with >300 benchmarks, 9 million data points
10. AtomVision	https://github.com/usnistgov/atomvision	Computer vision models and dataset for materials science, STEM/STM
11. AtomQC	https://github.com/usnistgov/atomqc	Quantum computation library for molecules and solids
12. Tb3Py	https://github.com/usnistgov/tb3py	Three-body tight-binding model for the periodic table
13. Solar	https://jarvis.nist.gov/jsolar	Solar cell materials design with DFT, AI

How to Get Started

github.com/JARVIS-Materials-Design/jarvis-tools-notebooks

JARVIS-Materials-Design / jarvis-tools-notebooks

Table of Contents

Collection of
Jupyter Notebooks
&
Recorded Videos

JARVIS-Tools Notebooks (Introduction)

The JARVIS-Tools Notebooks is a collection of Jupyter/ Google-Colab notebooks to provide on various methods for materials design. It consists of several types of applications such as

jarvis.nist.gov/events/

JARVIS

NIST

JARVIS-NIST Events

AIMS

QMMS

JARVIS-School

JARVIS

JARVIS-School is accompanied by
We plan to first g
topics such as:

nist.gov/news-events/events/2023/07/artificial-intelligence-materials-science-aims-workshop

0:00 / 5:49:39 1x NIST

2023 Artificial Intelligence for Materials Science (AIMS) Workshop

3 videos

20230725-27_AIMS_Day1 5:49:39

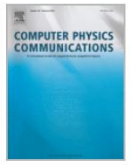
20230725-27_AIMS_Day2 4:44:20

20230725-27_AIMS_Day3 4:37:50

Feature engineering/descriptors

1. Element descriptors
2. MagPie
3. Coulomb matrix,
4. Ewald sum matrix,
5. sine matrix,
6. Many-body Tensor Representation (MBTR),
7. Atom-centered Symmetry Function (ACSF),
8. Smooth Overlap of Atomic Positions (SOAP),
9. Classical force-field inspired descriptors (CFID),
10. Sure independence screening and sparsifying operator (SISSO),…

Computer Physics Communications
Volume 247, February 2020, 106949



DScribe: Library of descriptors for machine learning in materials science ☆

Lauri Himanen [a], Marc O.J. Jäger [a], Eiaki V. Morooka [a], Filippo Federici Canova [a b], Yashasvi S. Ranawat [a], David Z. Gao [b c], Patrick Rinke [a f], Adam S. Foster [a d e]

Computational Materials Science
Volume 152, September 2018, Pages 60-69

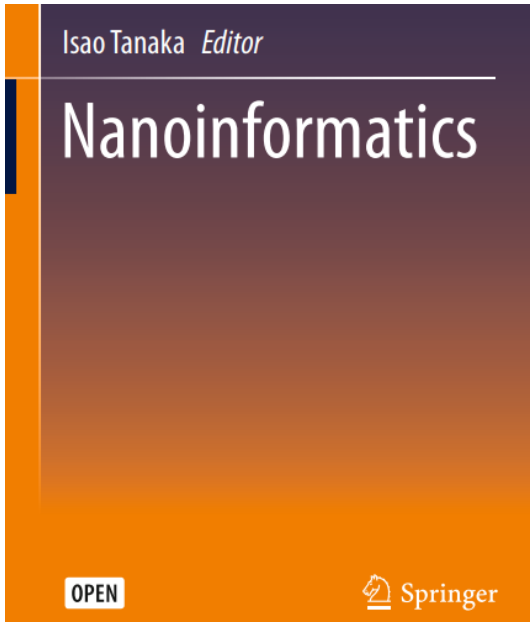
Matminer: An open source toolkit for materials data mining

Logan Ward [a b], Alexander Dunn [c d], Alireza Faghaninia [c], Nils E.R. Zimmermann [c], Saurabh Bajaj [c e], Qi Wang [c], Joseph Montoya [c], Jiming Chen [f], Kyle Bystrom [d], Maxwell Dylla [g], Kyle Chard [a b], Mark Asta [d], Kristin A. Persson [c], G. Jeffrey Snyder [g], Ian Foster [a b], Anubhav Jain [c]

Chemical fraction descriptors

	H	Li	Be	B	C	N	O	F	...
LiH	1	1	0	0	0	0	0	0	...
LiF	0	1	0	0	0	0	0	1	...
BeO	0	0	1	0	0	0	1	0	...
BN	0	0	0	1	0	1	0	0	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	...

Fig. 1.1 Binary elemental descriptors representing the presence of chemical elements. The number of binary elemental descriptors corresponds to the number of element types included in the training data



MagPie descriptors

Element Property statistics of Magpie	Additional Predictors of Magpie	Added Predictors in this work
Atomic Number	Stoichiometry p-norm (p = 0,2,3,5.7)	Total Atom Number
Mendeleev Number	Elemental Fraction	Maximum Atom Number
Atomic Weight	Fraction of Electrons in each Orbital	Minimum Atom Number
Melting Temperature	Band Center	Average Atom Number
Periodic Table Row and Column	Ion Property (possible to form ionic compound, ionic charge)	Specific Value
Covalent Radius		Atom Number Variance
Electronegativity		
The number of Valence e in each orbital(s, p. d, f, total)		
The number of unfilled e in each orbital (s, p. d, f, total)		
Ground State Volume		
Ground State Band Gap Energy		
Ground State Magnetic Moment		
Space Group Number of elements		

https://doi.org/10.1016/j.commatsci.2021.110686

npj | computational materials

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nature › npj computational materials › articles › article

Article | Open access | Published: 26 August 2016

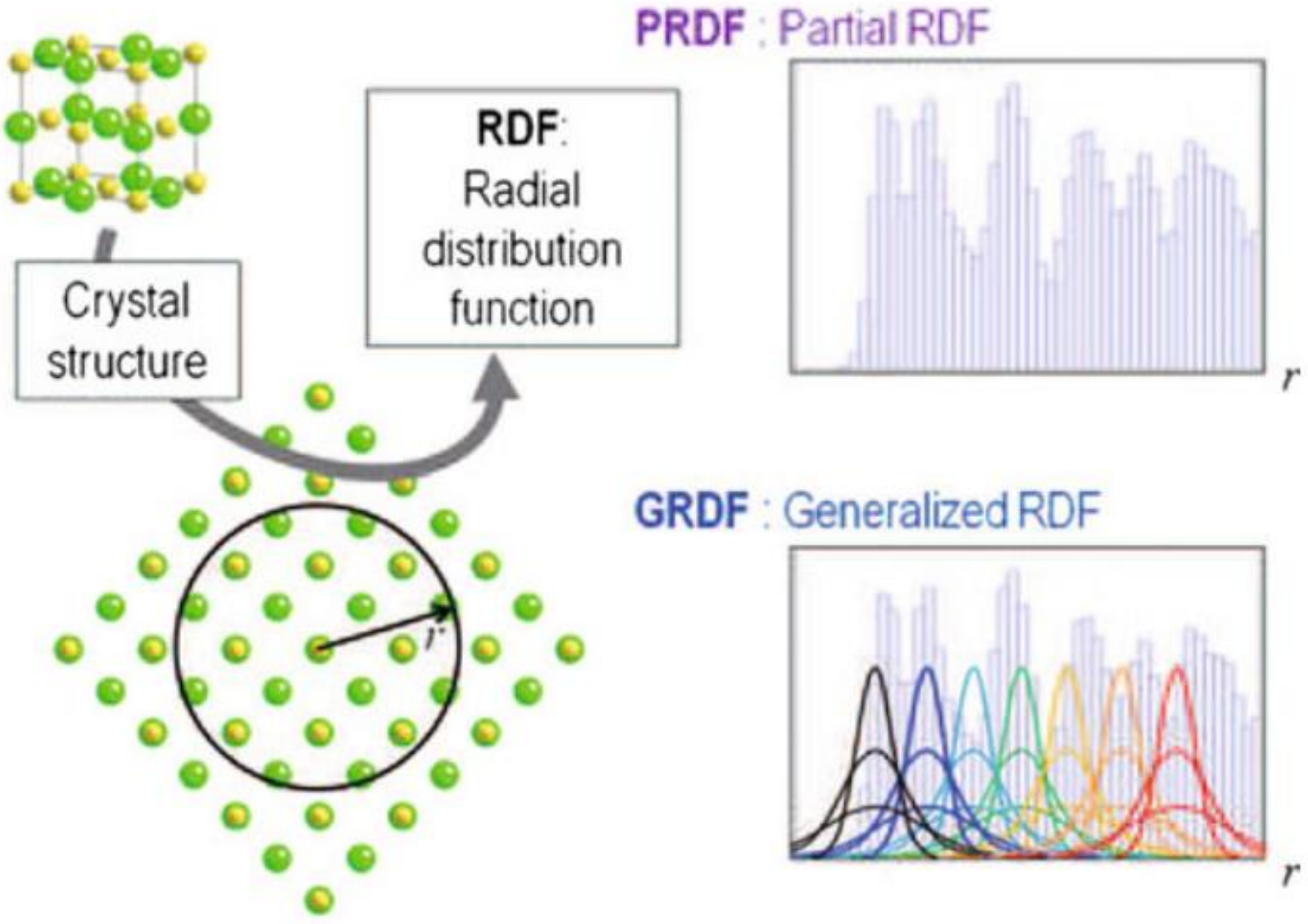
A general-purpose machine learning framework for predicting properties of inorganic materials

Logan Ward, Ankit Agrawal, Alok Choudhary & Christopher Wolverton

npj Computational Materials **2**, Article number: 16028 (2016) | Cite this article

60k Accesses | **1067** Citations | **18** Altmetric | Metrics

Structural descriptors (RDF/PRDF)



Coulomb matrix descriptors

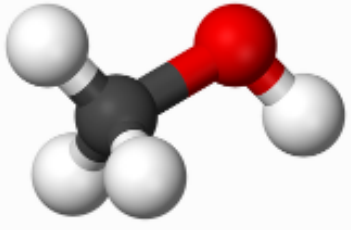
Coulomb matrix is calculated with the equation below.

$$M_{ij}^{\text{Coulomb}} = \begin{cases} 0.5 Z_i^{2.4} & \text{for } i = j \\ \frac{Z_i Z_j}{R_{ij}} & \text{for } i \neq j \end{cases}$$

The diagonal elements can be seen as the interaction of an atom with itself and are essentially a polynomial fit of the atomic energies to the nuclear charge Z_i. The off-diagonal elements represent the Coulomb repulsion between nuclei i and j.

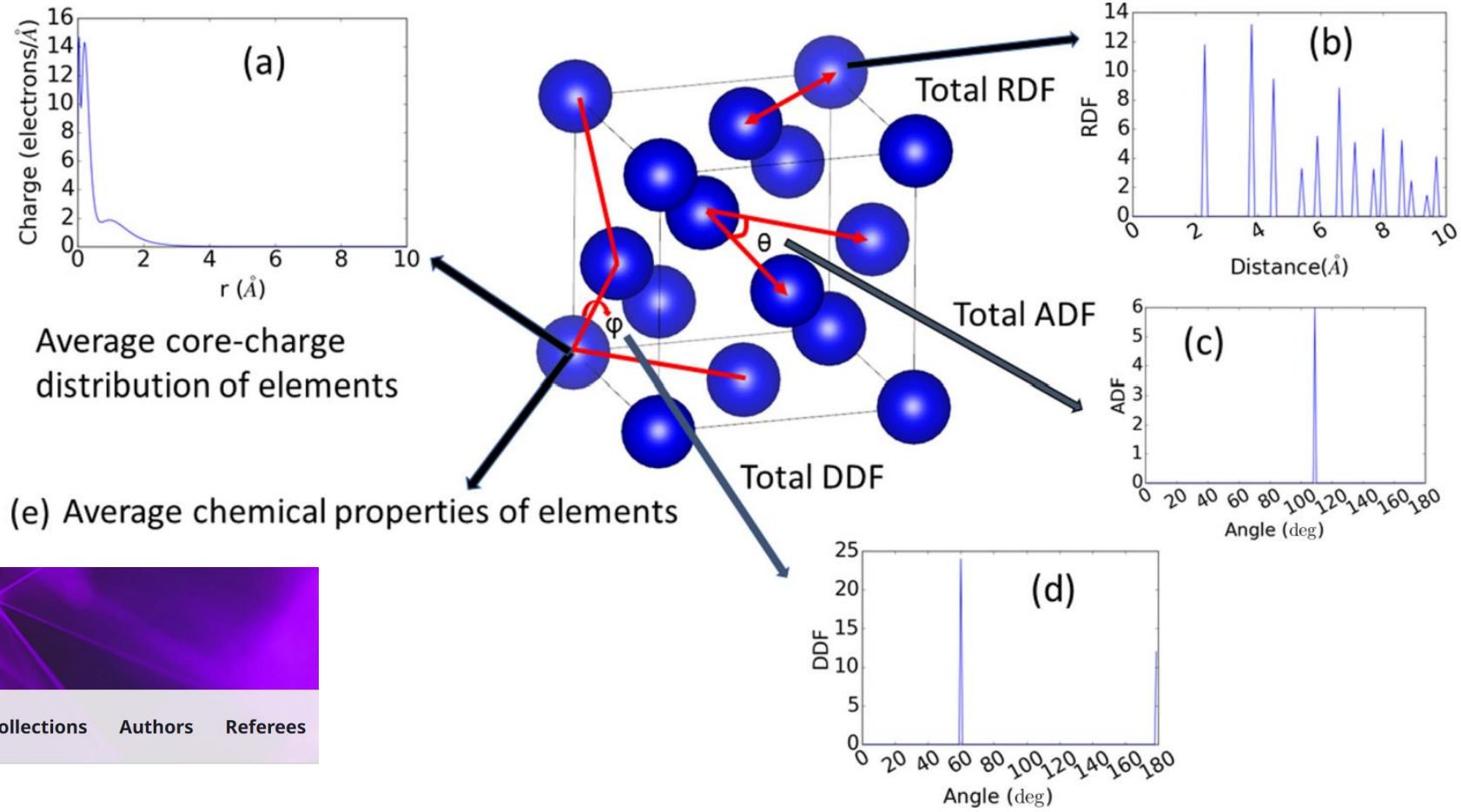
Let's have a look at the CM for methanol:

https://singroup.github.io/dscribe/0.3.x/tutorials/coulomb_matrix.html



$$\begin{bmatrix} 36.9 & 33.7 & 5.5 & 3.1 & 5.5 & 5.5 \\ 33.7 & 73.5 & 4.0 & 8.2 & 3.8 & 3.8 \\ 5.5 & 4.0 & 0.5 & 0.35 & 0.56 & 0.56 \\ 3.1 & 8.2 & 0.35 & 0.5 & 0.43 & 0.43 \\ 5.5 & 3.8 & 0.56 & 0.43 & 0.5 & 0.56 \\ 5.5 & 3.8 & 0.56 & 0.43 & 0.56 & 0.5 \end{bmatrix}$$

CFID Descriptors



Physical Review Materials

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Machine learning with force-field-inspired descriptors for materials: Fast screening and mapping energy landscape

Kamal Choudhary, Brian DeCost, and Francesca Tavazza

Other Descriptors

Behler-Parinello

Behler-Parinello (BP) also called "Gaussian" fingerprints are local fingerprints based on symmetry functions. Two of such symmetry functions are given by the radial and angular componenets G^{rad} and G^{ang} below where summations run over all neighbors j and k separated by distances R_{ij} and R_{ik} with respect to atom i within a cutoff distance R_c around i. θ_{ijk} is the angle between atoms $i, jandk$. η, R_s, λ and ζ are parameters whose values are chosen by the user. f_c is a cutoff function used to ensure a smooth transition to zero at the R_c. For more information, see: [BP]

$$G_i^{rad} = \sum_j e^{-\eta(R_{ij}-R_s)^2} f_c(R_{ij})$$

$$G_i^{ang} = 2^{1-\zeta} \sum_{j,k\neq i} (1+\lambda\cos\theta_{ijk})^{\zeta} e^{-\eta(R_{ij}^2+R_{ik}^2+R_{jk}^2)^2} f_c(R_{ij}) f_c(R_{ij}) f_c(R_{ij})$$

$$f_c = \begin{cases} 0.5[\cos(\frac{\pi R_{ij}}{R_c})+1] & \text{for} \quad R_{ij} \leq R_c \\ 0 & \text{for} \quad R_{ij} > R_c \end{cases}$$

AGNI

The [AGNI] method was developed as a framework for machine learning force field development i which the forces are calculated directly without going through energy predictions. The associated fingerprint is given by $V_{i,\alpha,k}$ below where α denotes the direction (x,y or z) of the force between atoms i and j separated by distance r_{ij}. The parameter w corresponds to the width of Gaussians placed at positions a_k within a cutoff distance R_c. Similarly to the BP fingerprint, f_c is the cutofff function ensuring a smooth transition to zero at Rc.

$$V_{i,\alpha,k} = \sum_{j\neq i} \frac{r_{ij}^{\alpha}}{r_{ij}} \frac{1}{\sqrt{2\pi w}} e^{-0.5(\frac{r_{ij}-a_k}{w})^2} f_c(r_{ij})$$

Bispectrum

Bispectrum fingerprints for representaion of chemical environments were proposed by Bartok et al. and are based on teh decomposition of a local atomic density function with respect to 4D spherical harmonics. The bispecturm representation is then build based on the coefficients $c^j_{m'm}$ of the decomposition given below. For more information, please consult the original paper on the development of [Bispectrum] fingerprints.

$$B_{j_1,j_2,j} = \sum_{m_1',m_1=-j_1}^{j_1} \sum_{m_2',m_2=-j_2}^{j_1} \sum_{m',m=-j}^{j} c^j_{m'm} C^{jm}_{j_1 m_1 j_2 m_2} C^{jm'}_{j_1 m_1' j_2 m_2'} c^{j_1}_{m_1' m_1} c^{j_2}_{m_2' m_2}$$

Zernike

Zernike fingerprints are similar to Bispectrum fingerprints in the sense that they are based on decomposition of a local atomic density wrt basis sets. However, Zernike fingerprints are based on decomposition wrt zernike polynomials and 3D spherical harmonics. The general formula is given below. Please consult this paper which describes the [Zernike] method.

$$\rho(\tilde{r},\theta,\phi) = \sum_{n=0}^{\inf} \sum_{l} \sum_{m=-l}^{l} c_{nl}^m Z_{nl}^m(\tilde{r},\theta,\phi) \quad \text{for} \;\; n-l \geq 0$$

https://seing.readthedocs.io/en/latest/theory.html

Comparison of Descriptors

```
# Convert my_data to numpy array using CFID-Chem, Magpie and elemental fraction descriptors

X_cfid = []
X_Mag = []
X_elff = []

Y = []
IDs = []

for ii, i in enumerate(my_data):
    comp = i[0]
    desc_magpie,magpie_names = get_chem_only_descriptors(formula=comp, source="magpie")
    val = i[1]
    X_Mag.append(desc_magpie)
    Y.append(val)
    IDs.append(ii)

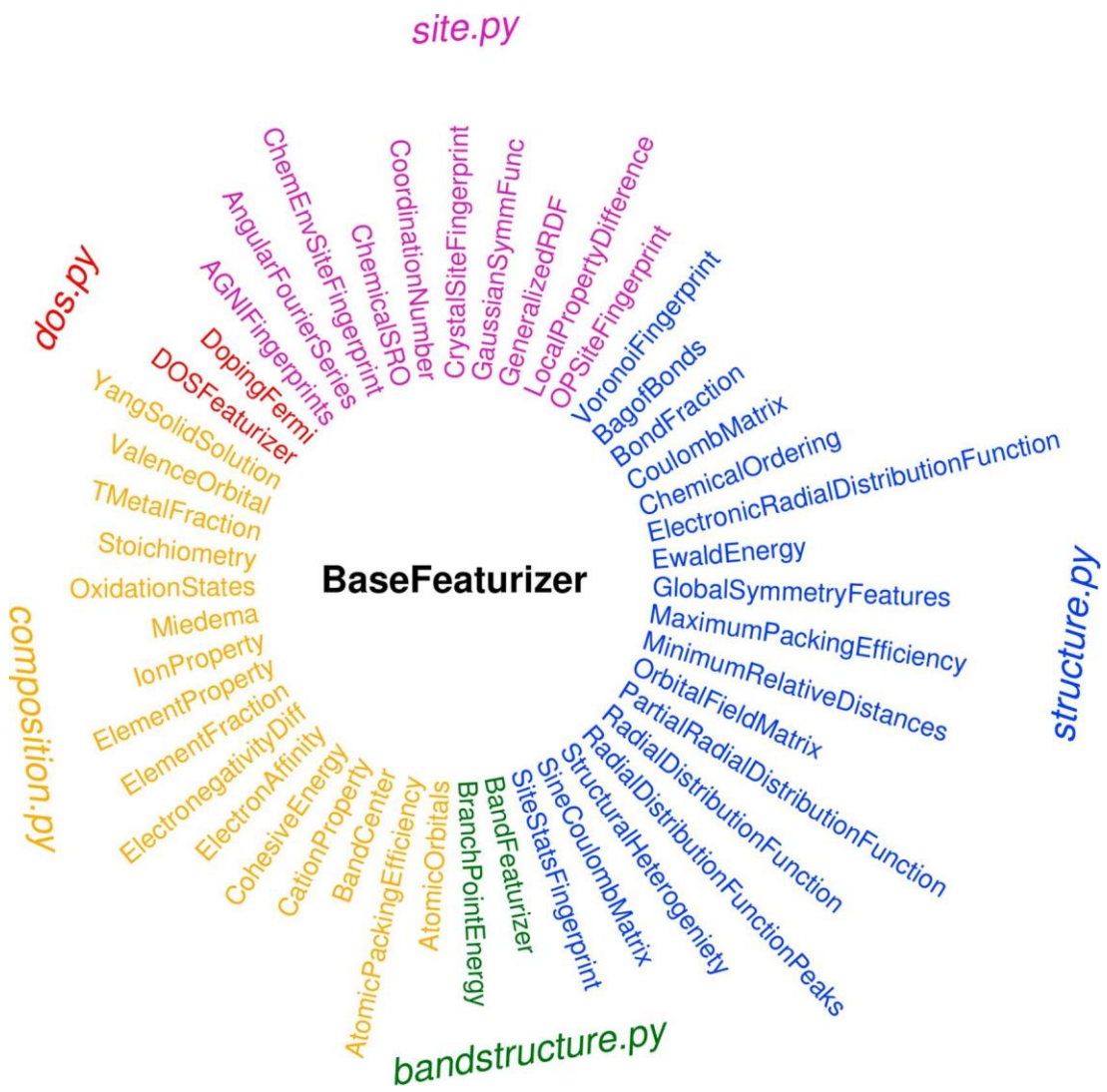
X_Mag = np.array(X_Mag)

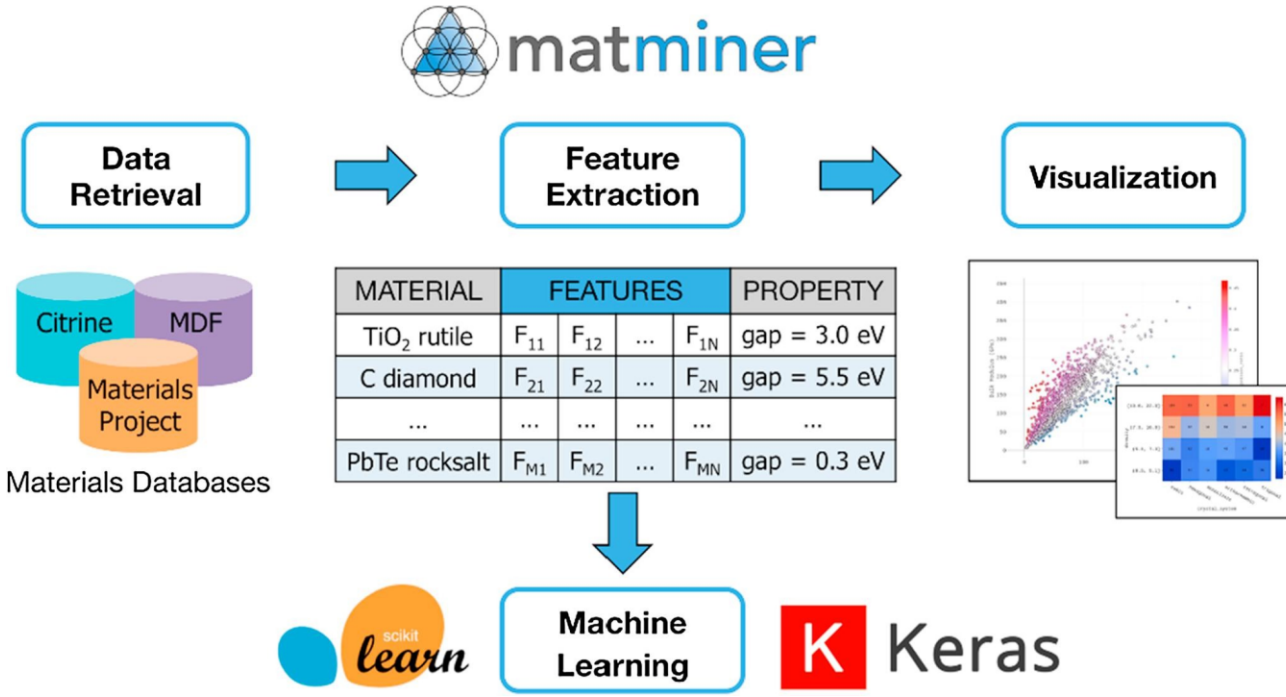
Y = np.array(Y).reshape(-1, 1)

'''
Print out the mean absolute deviation, which captures the spread of values in
the target property distribution
'''
IDs = np.array(IDs)
mad = mean_absolute_deviation(Y)
print("MAD:", mad)
```

jarvis-tools-notebooks (AI. 2)

MatMiner


site.py
structure.py
bandstructure.py
composition.py
dos.py
BaseFeaturizer
ChemEnvSiteFingerprint
AngularFourierSeries
AGNIFingerprints
DopingFermi
DOSFeaturizer
YangSolidSolution
ValenceOrbital
TMetalFraction
Stoichiometry
OxidationStates
Miedema
IonProperty
ElementProperty
ElementFraction
ElectronegativityDiff
ElectronAffinity
CohesiveEnergy
CationProperty
BandCenter
AtomicPackingEfficiency
AtomicOrbitals
BranchPointEnergy
BandFeaturizer
SiteStatsFingerprint
SineCoulombMatrix
StructuralHeterogeniety
RadialDistributionFunctionPeaks
RadialDistributionFunction
PartialRadialDistributionFunction
OrbitalFieldMatrix
MinimumRelativeDistances
MaximumPackingEfficiency
GlobalSymmetryFeatures
EwaldEnergy
ElectronicRadialDistributionFunction
ChemicalOrdering
CoulombMatrix
BondFraction
BagofBonds
VoronoiFingerprint
OPSiteFingerprint
LocalPropertyDifference
GeneralizedRDF
GaussianSymmFunc
CrystalSiteFingerprint
CoordinationNumber
ChemicalSRO


matminer
Data Retrieval
Feature Extraction
Visualization
Citrine
MDF
Materials Project
Materials Databases
MATERIAL
FEATURES
PROPERTY
TiO2 rutile
F11
F12
...
F1N
gap = 3.0 eV
C diamond
F21
F22
...
F2N
gap = 5.5 eV
...
...
...
...
...
...
PbTe rocksalt
FM1
FM2
...
FMN
gap = 0.3 eV
scikit learn
Machine Learning
Keras

Day 3 Hands on

AI 1 ML Sklearn Steel Fatigue

AI 2 ML_Chem_Formula_Descriptors

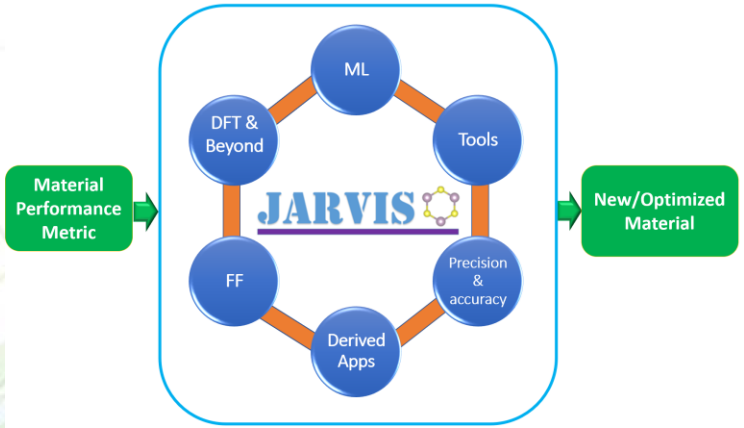
AI 3 Simple_Machine_learning_training_example_with_CFID_descriptors

AI 5 JARVIS_CFID_LightGBM_GPUvsCPU

Materials Informatics: Fingerprints, Graph Neural Networks, and Transformers Based Models for Materials Design

Kamal Choudhary
Staff Scientist
NIST, Gaithersburg, MD, USA

Jan 20-25, 2025



https://jarvis.nist.gov

Joi[illegible] Integ[illegible]

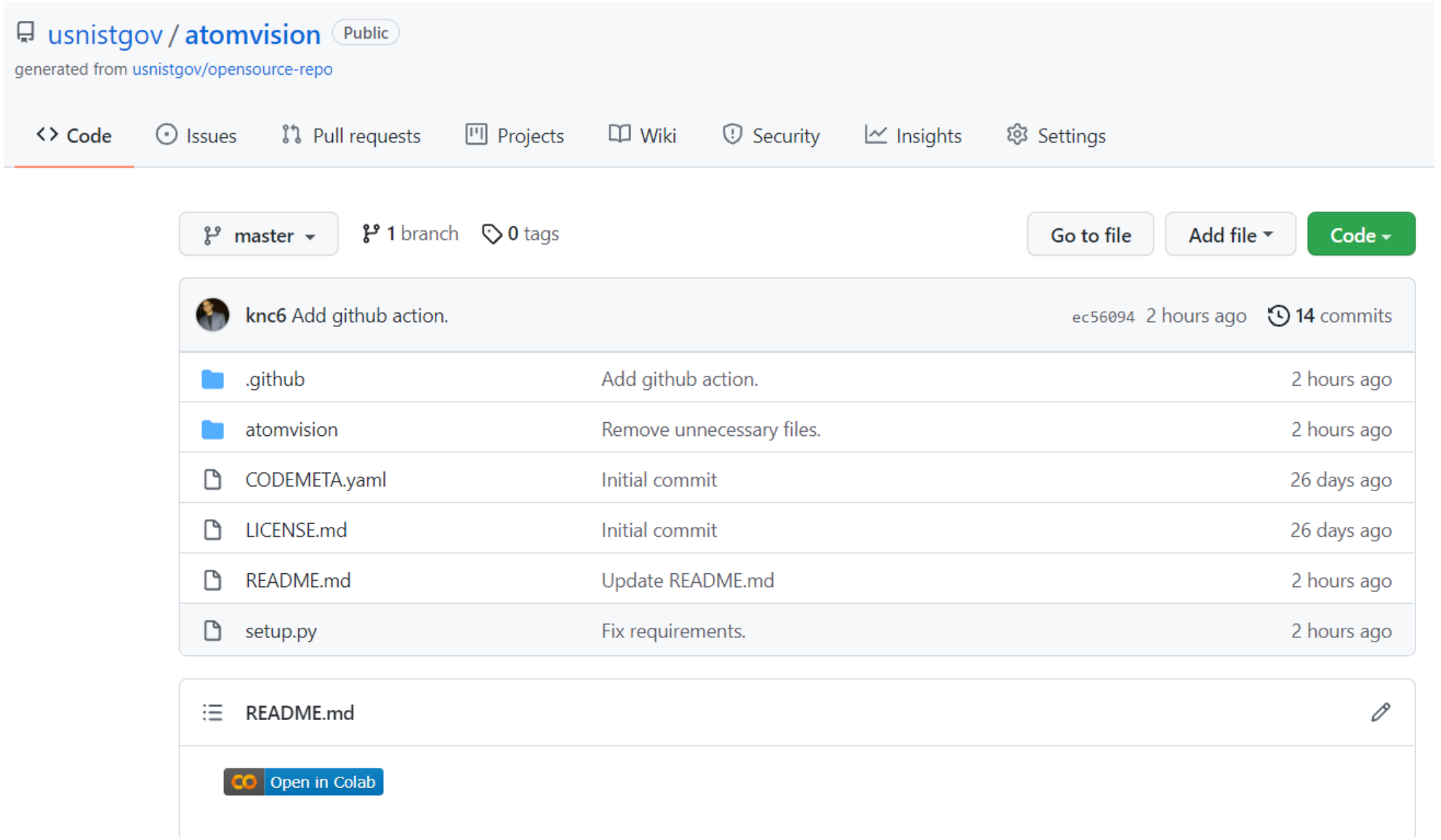
NIST NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Day 4

- Deep learning models (CNN, GAN, GNN, GPT,…)
- AtomVision
- ALIGNN
- ChemNLP
- AtomGPT
- DiffractGPT
- JARVIS-Leaderboard
- Benchmarking and reproducibility

AtomVision

A deep learning framework for atomistic image data



AtomVision

A deep learning framework for atomistic image data

usnistgov / atomvision Public

generated from usnistgov/opensource-repo

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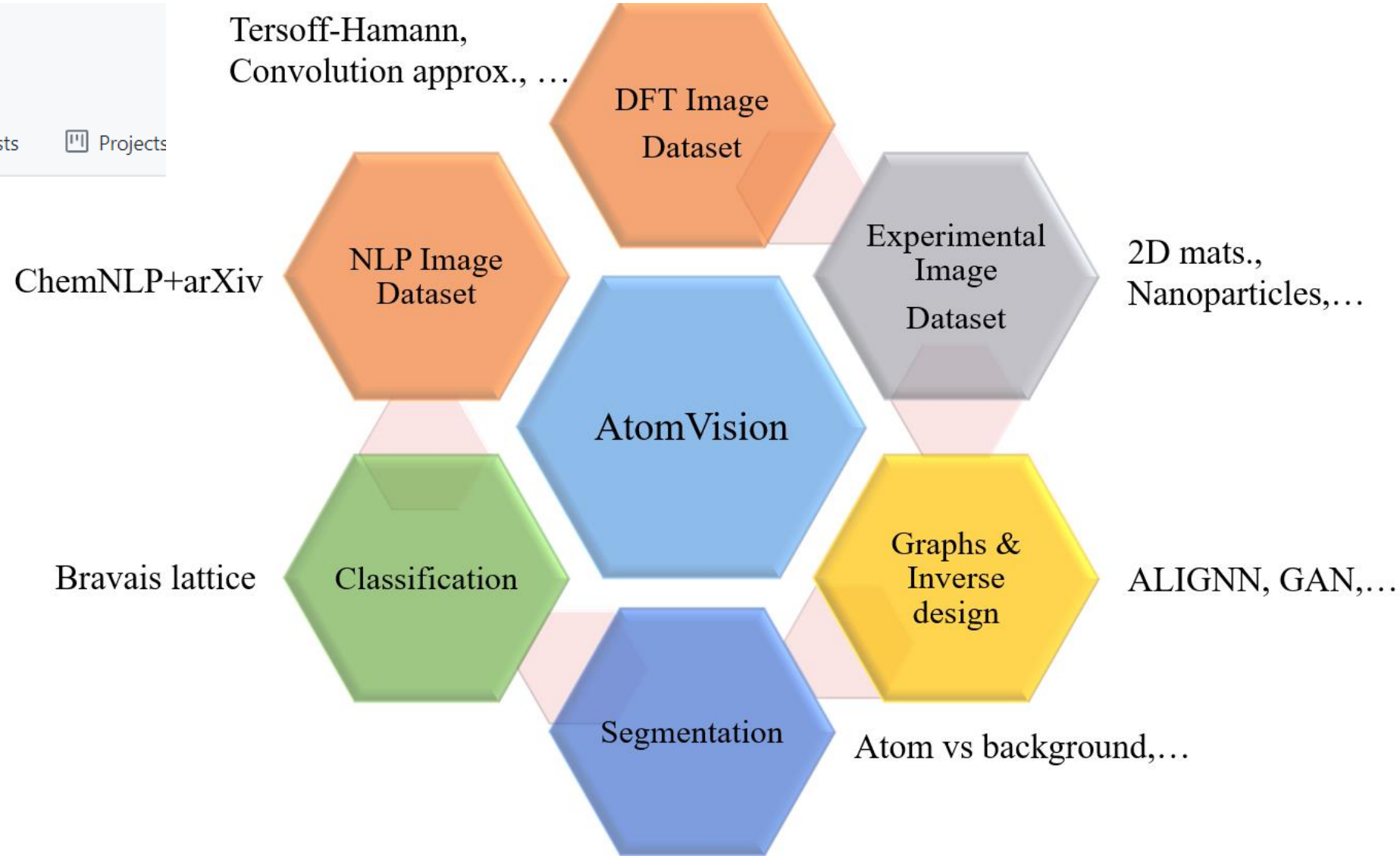
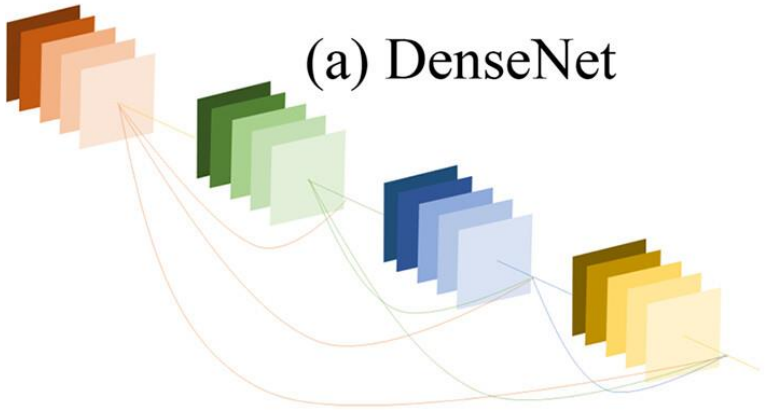
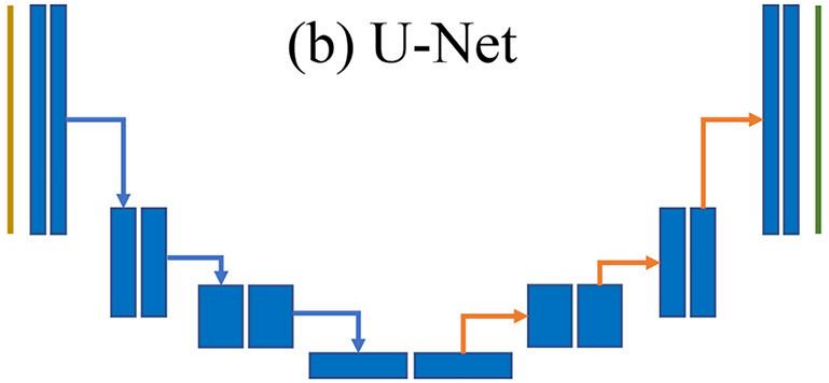
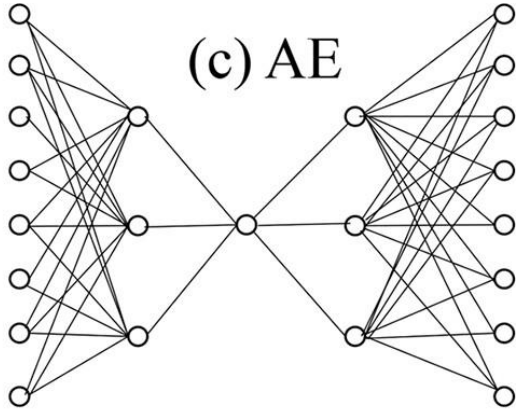


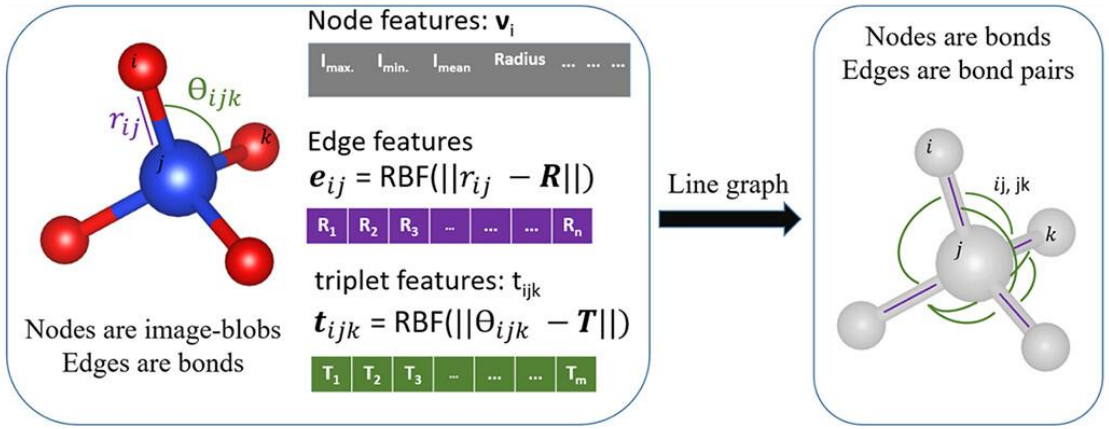
AtomVision



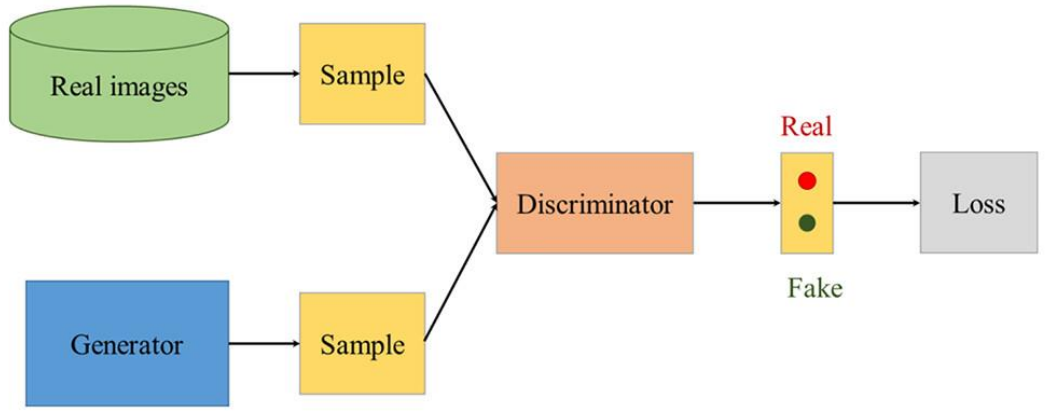




(d) ALIGNN



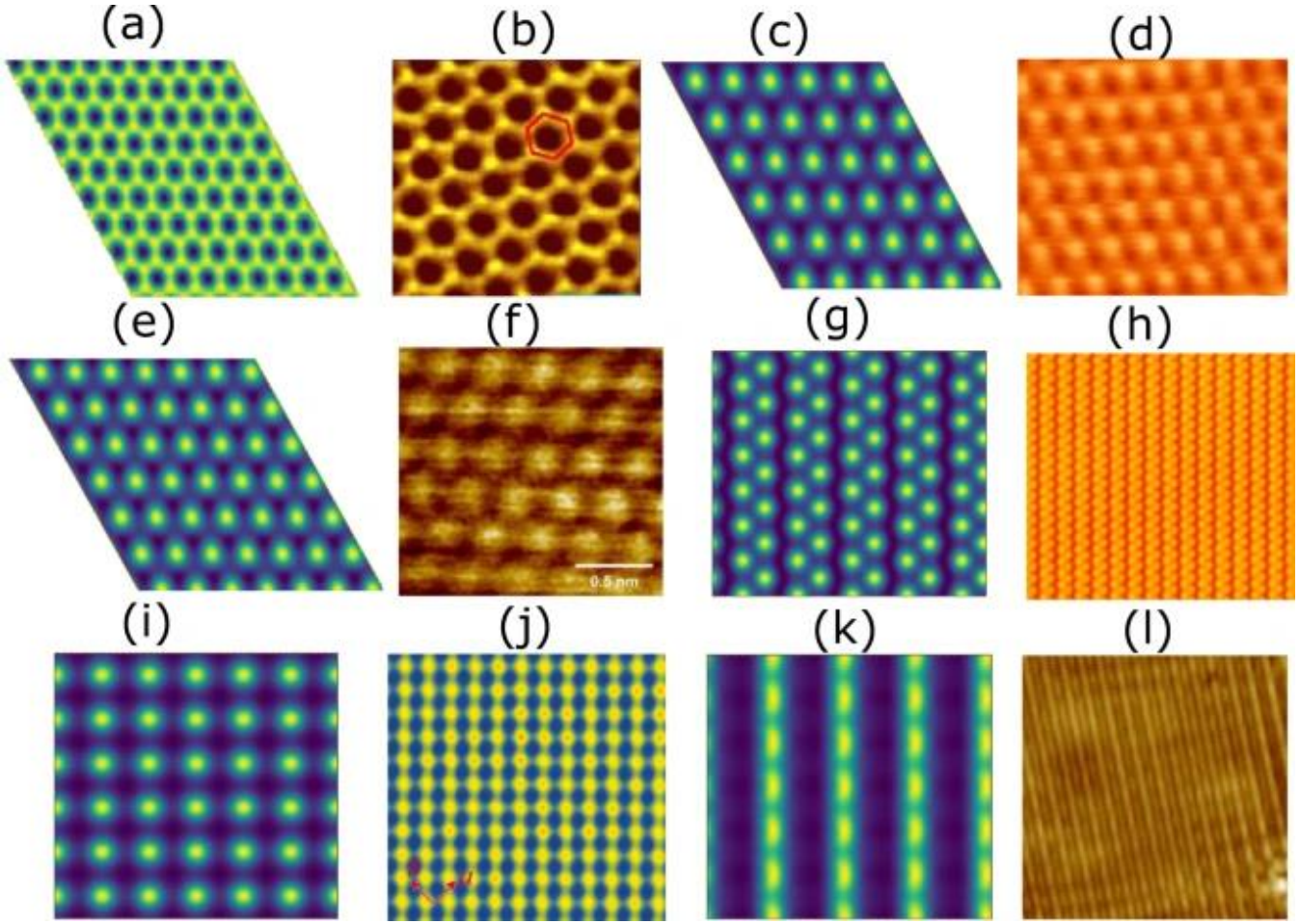
(e) SRGAN



Scanning Tunneling Microscope Image

Tersoff-Hamman approach, constant **height**/current images

Tunneling current is proportional to the integrated local density of states (ILDOS)



$$n(r, E) = \sum_{\mu} |\psi_{\mu}(r)|^2 \delta(\varepsilon_{\mu} - E)$$

$$I(r, V) \propto \int_{E_F}^{E_F+eV} dE\, n(r, E)$$

nature › scientific data › data descriptors › article

Data Descriptor | Open Access | Published: 11 February 2021

Computational scanning tunneling microscope image database

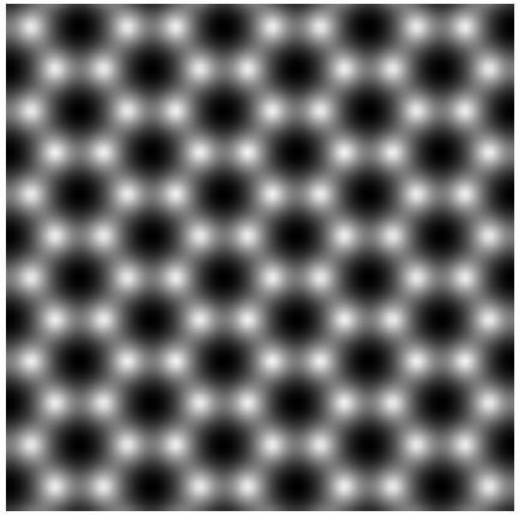
Kamal Choudhary, Kevin F. Garrity, Charles Camp, Sergei V. Kalinin, Rama Vasudevan, Maxim Ziatdinov & Francesca Tavazza

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

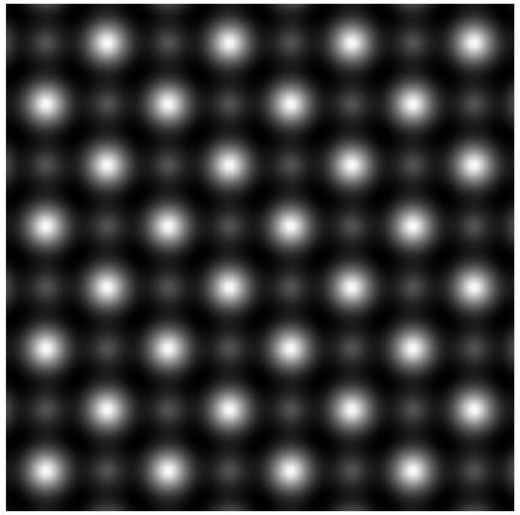
Scanning Transmission Electron Microscope Image

Convolution approximation: accurate for **thin films** mainly
Based on Rutherford scattering model

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



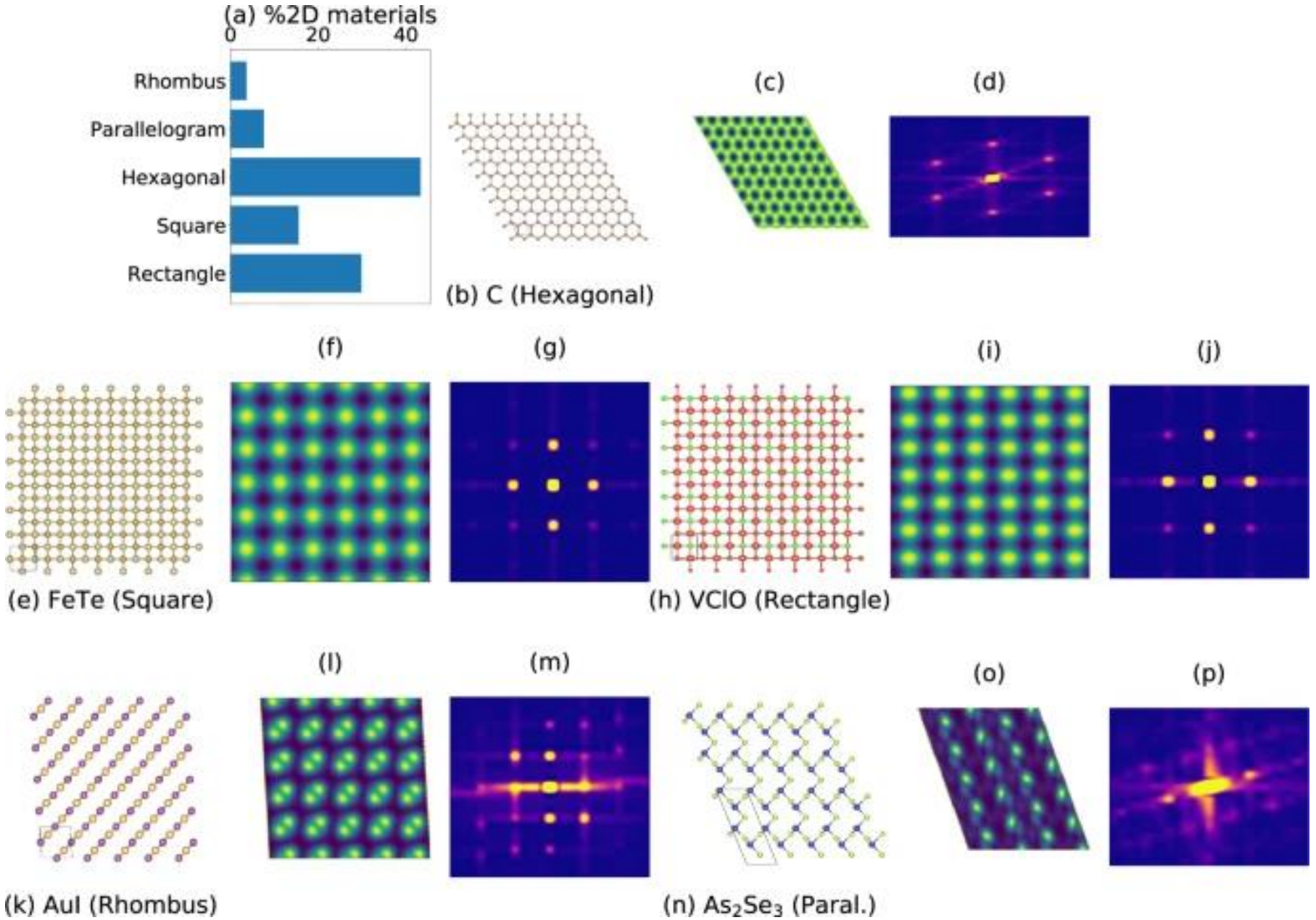
C: JVASP-667



FeTe: JVASP-6667

PPdSe: JVASP-6316

2D Lattice Classification



T-SNE Plot

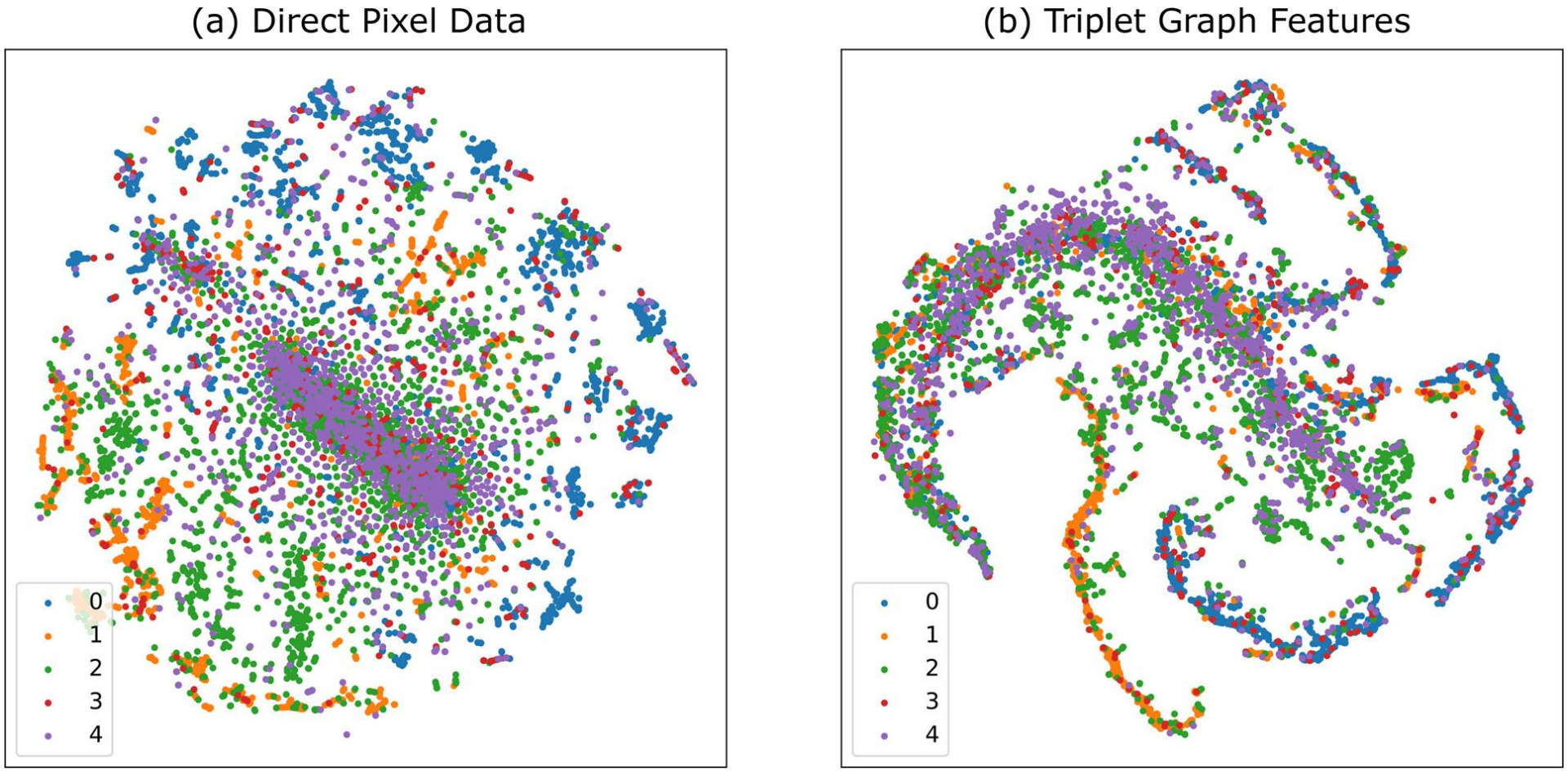
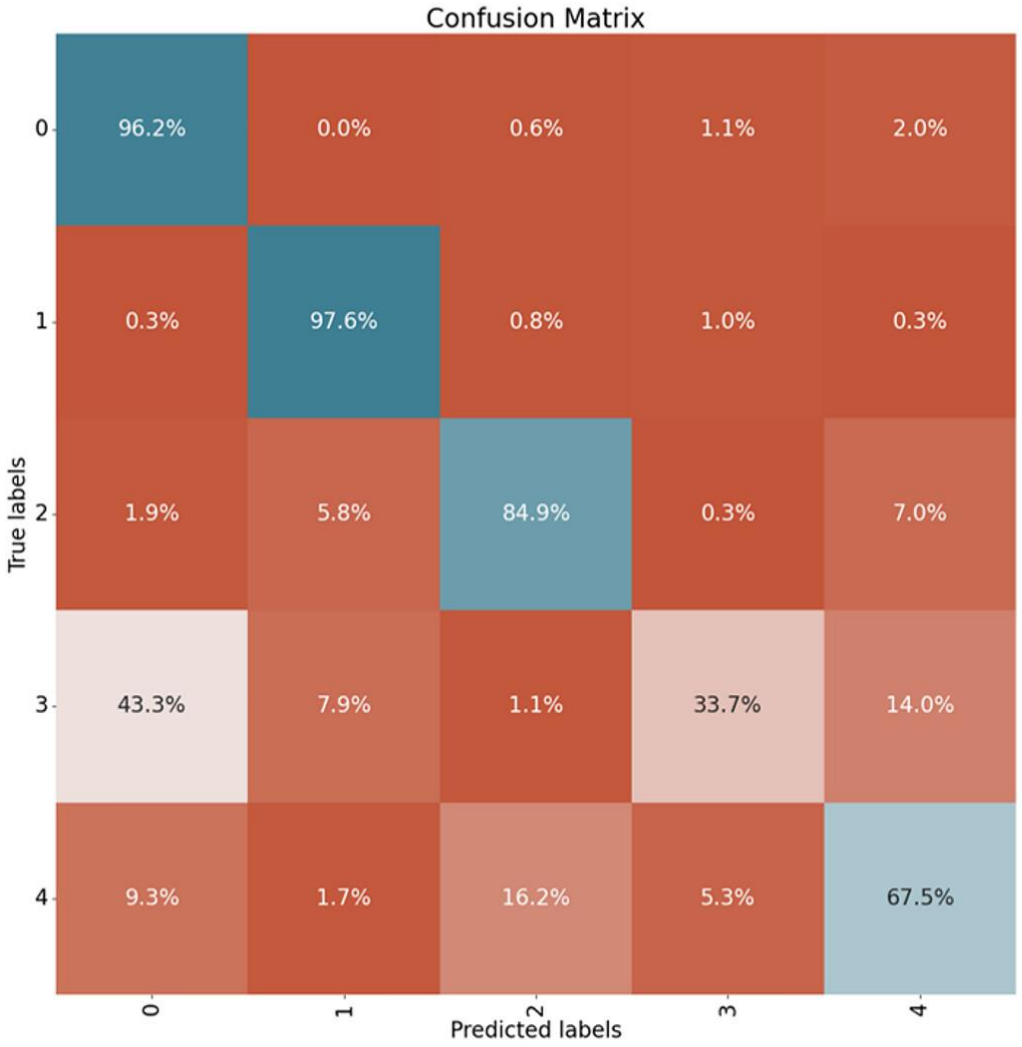


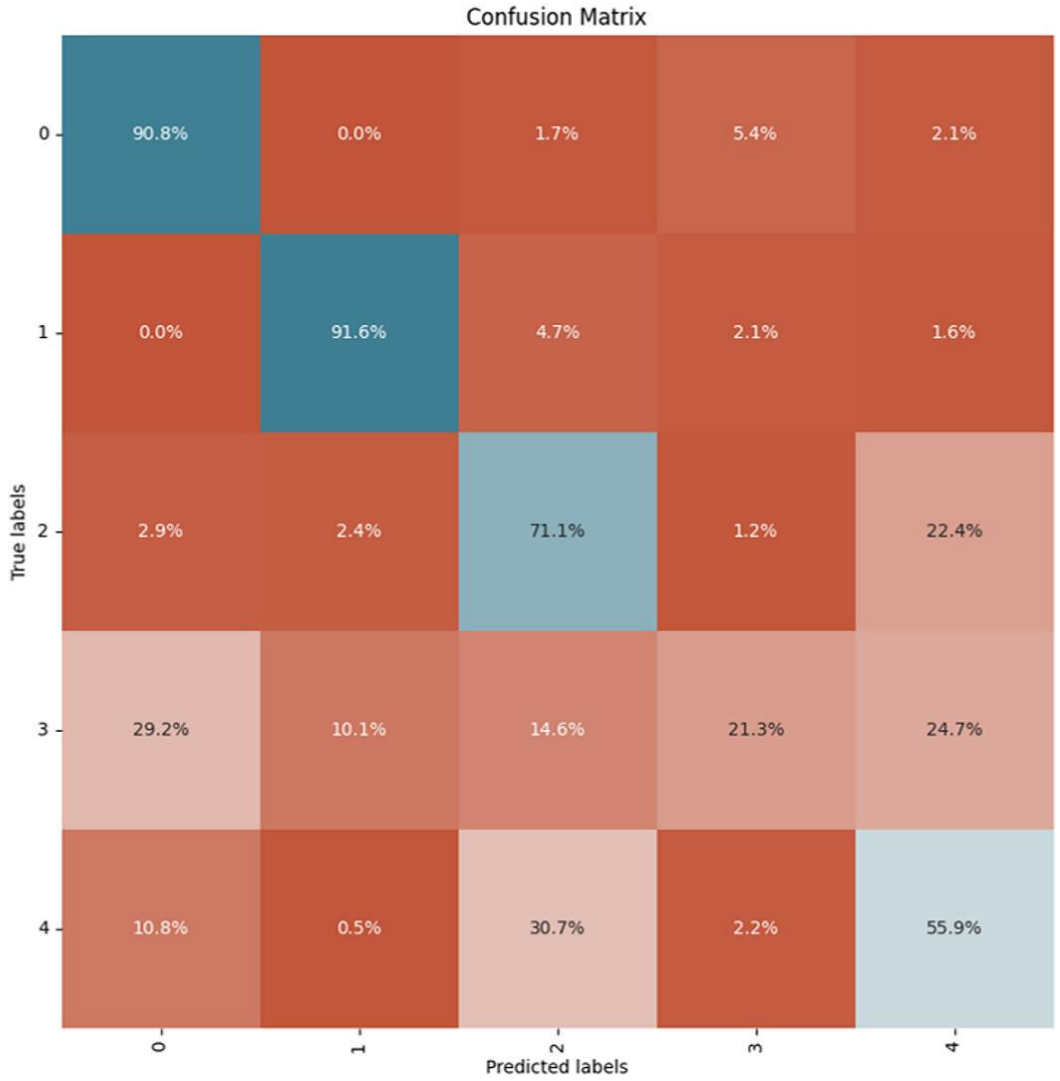
Figure 5. t-SNE visualization of the samples in the combined data set including the JARVIS-DFT-2D and C2DB databases. In panel (a), the samples are featurized directly using the 256 × 256 pixel image intensity data. In contrast, in panel (b), the samples are featurized using their triplet (bond angle cosine) features in graph construction. The distribution of triplet features is expressed as a 200-bin histogram ranging from −1 to 1. Here, we denote hexagonal, square, rectangle, rhombus, and parallelogram classes as 0, 1, 2, 3, and 4, respectively. We observe clusters of individual classes in both t-SNE figures.

CNN and GNN Classifier

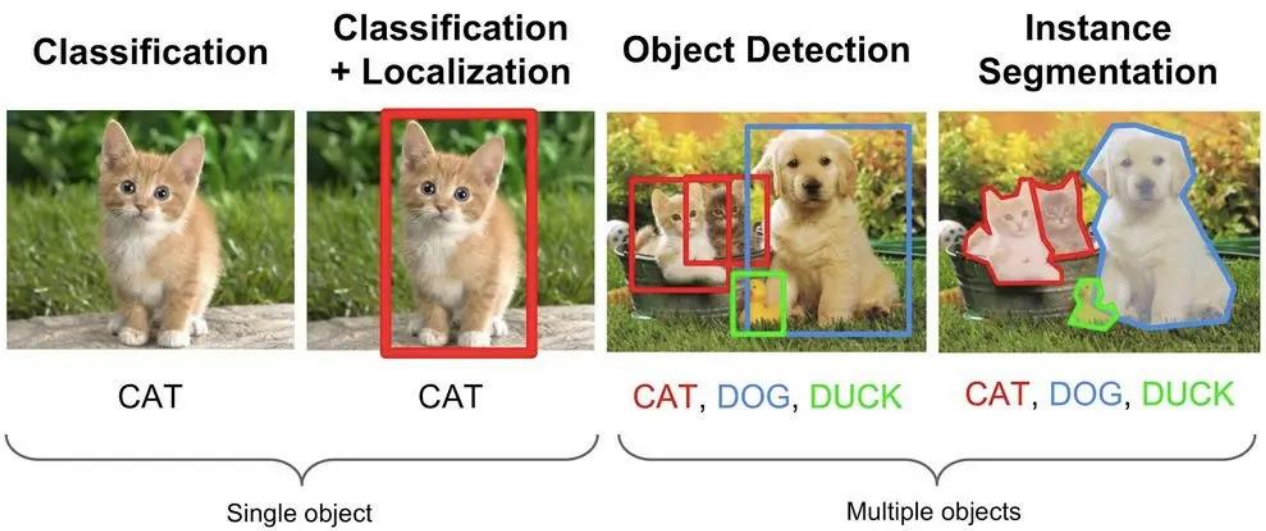
(a) DenseNet Classifier

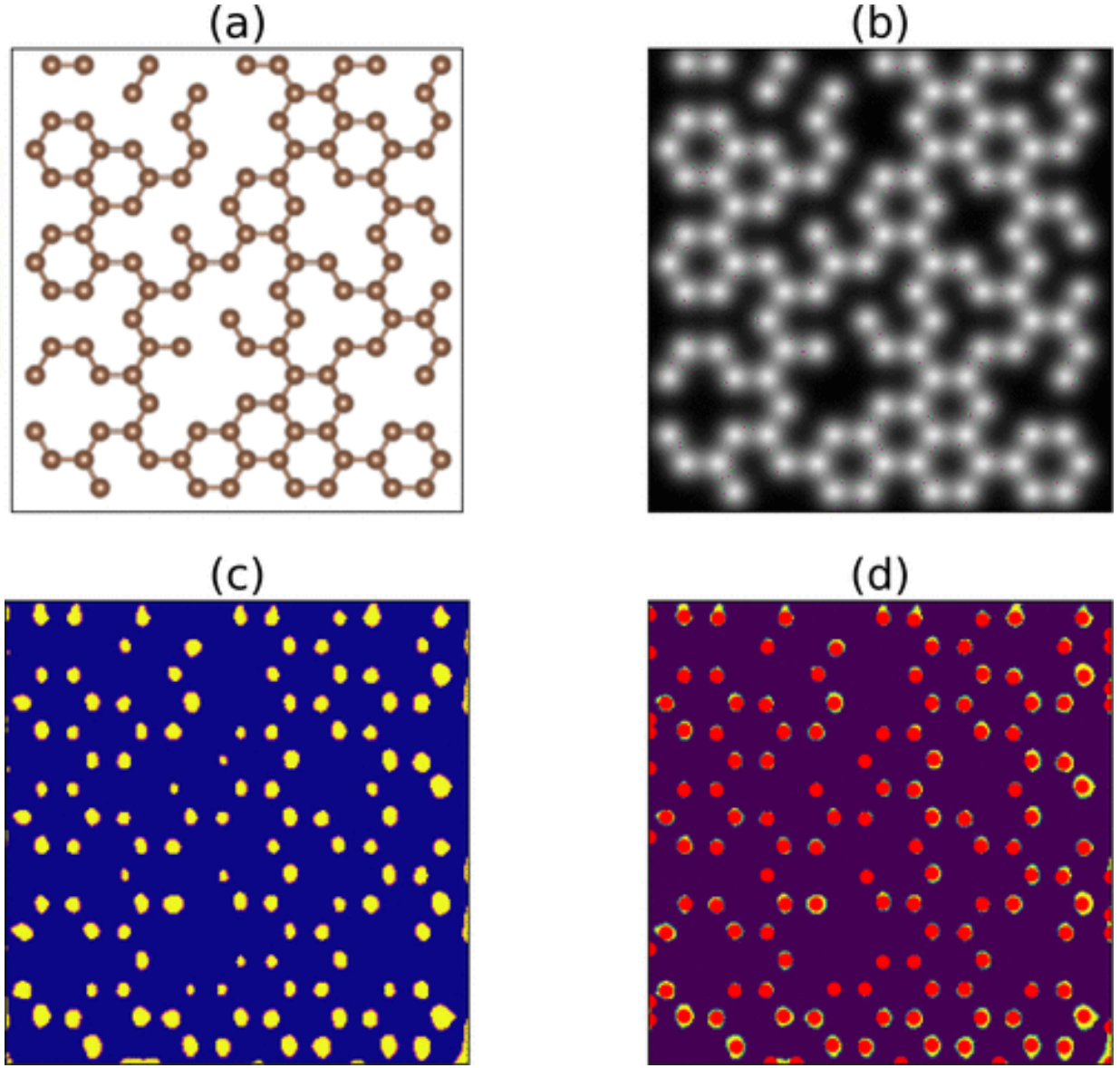


(b) ALIGNN Classifier



Semantic segmentation





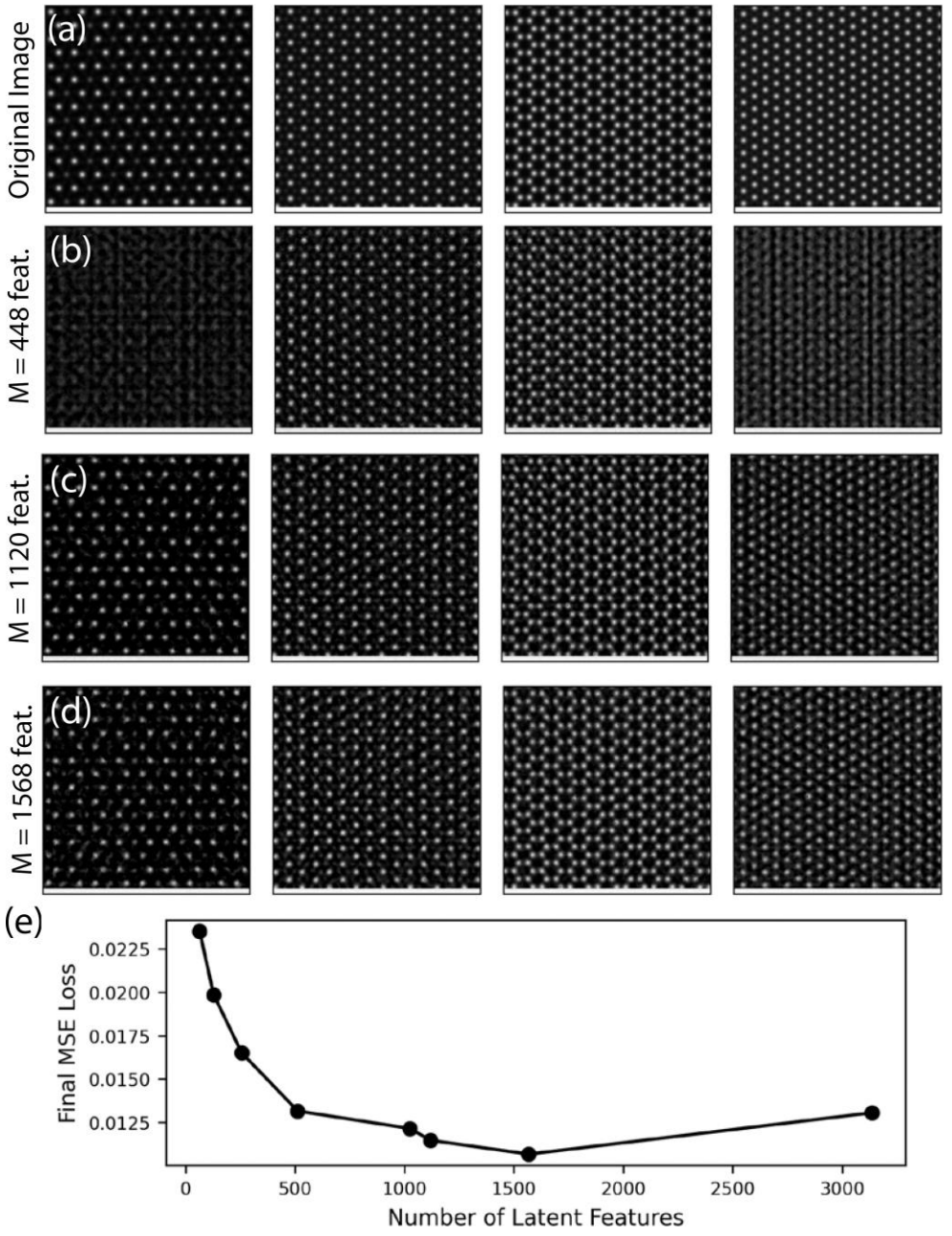
Application of semantic segmentation model to identify atoms and background from defective graphene system: (a) generation of the atomic structure for defective graphene (JVASP-667) with vacancies using JARVIS-Tools, (b) STEM image generation for the atomic structure, (c) use of the semantic segmentation model, and (d) use of the blob detection algorithm to find the number of atoms.

AutoEncoders

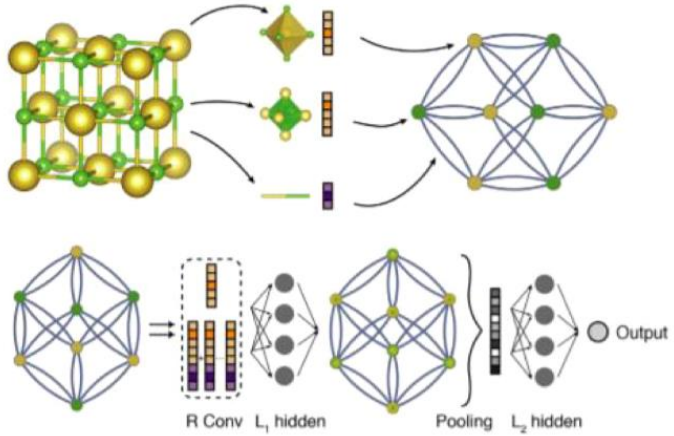
The autoencoder reconstructed images while varying the dimensionality of the latent space (M).

Performance of the model, as determined by MSE loss and the visual quality of reconstructed images, improves when increasing from 448 to 1120 latent features but does not significantly change when increasing to 1568 latent features.

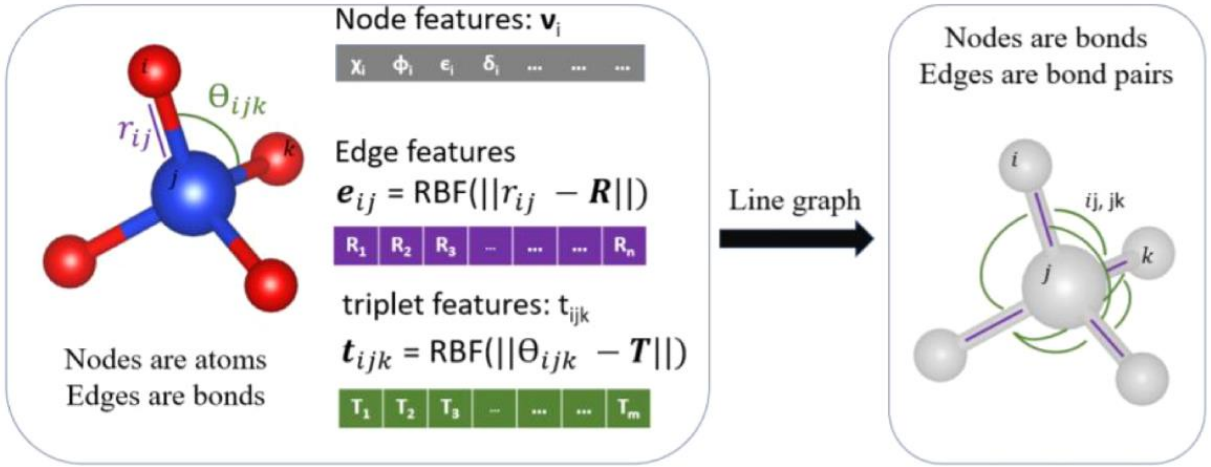
The MSE loss starts to increase at a larger number of latent features.



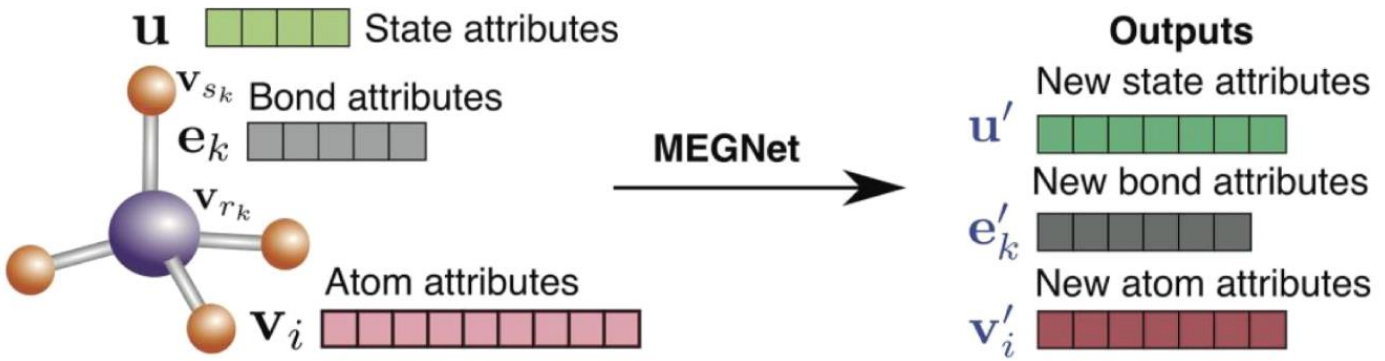
Graph Neural Networks



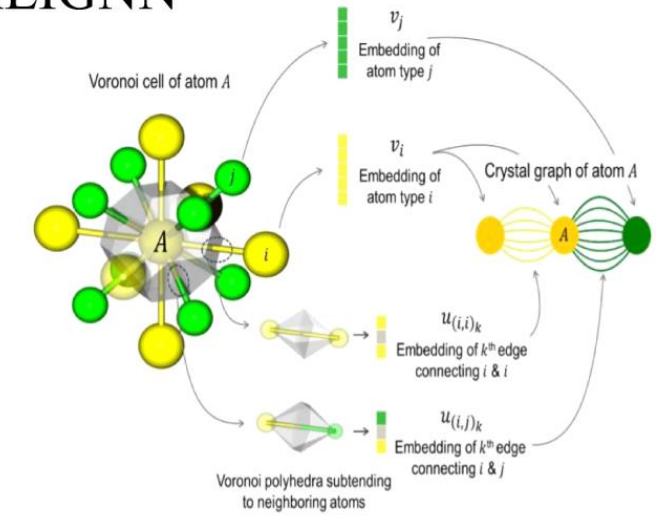
(a) CGCNN



(b) ALIGNN



(c) MEGNet



(d) iCGCNN

ALIGNN

Atomistic Line Graph Neural Network

github.com/usnistgov/alignn

usnistgov / alignn

Type / to

Code | Issues 23 | Pull requests 5 | Discussions | Actions | Proje

alignn Public

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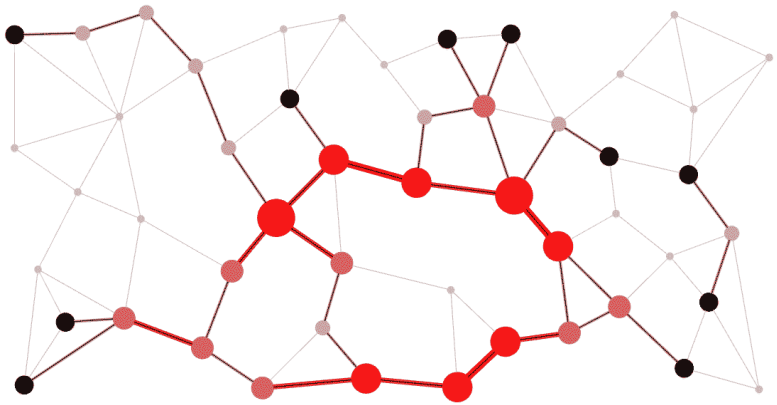

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Atomistic Line Graph Neural Network for improved materials property predictions

Kamal Choudhary & Brian DeCost

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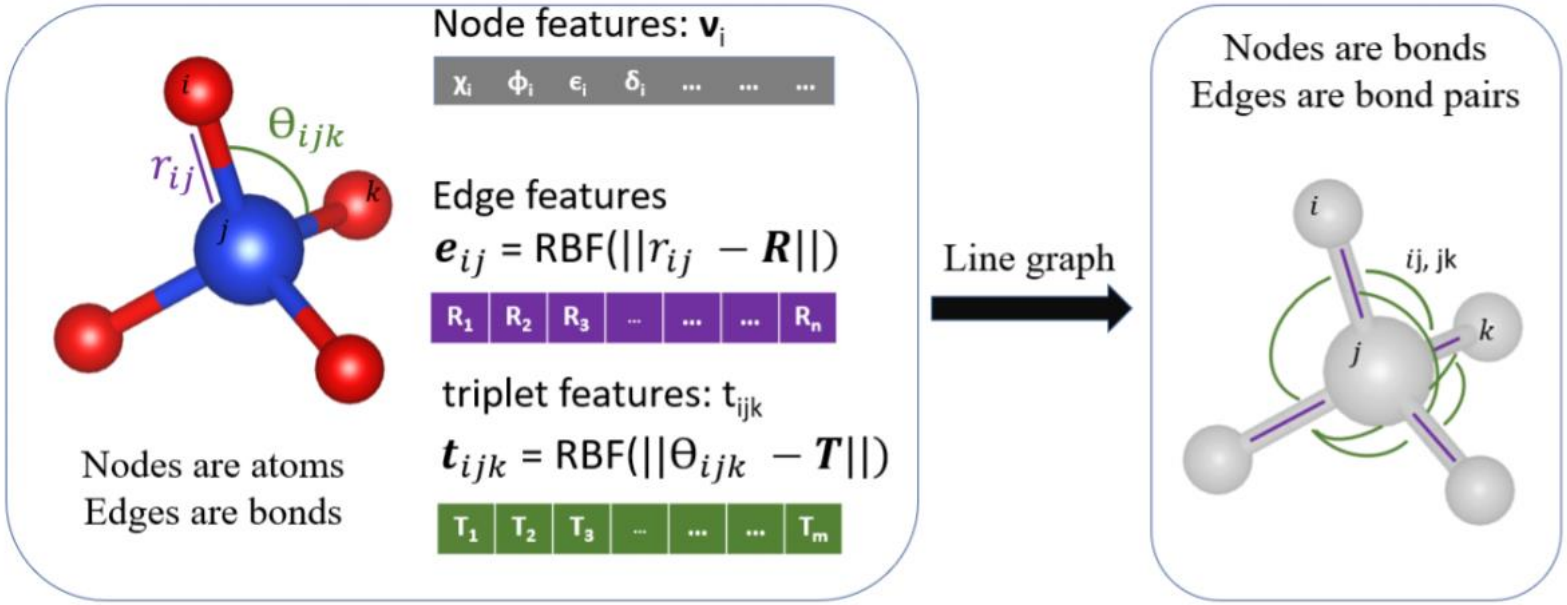
Unified graph neural network force-field for the periodic table: solid state applications

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

Atomistic Graph & 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



- Graph level prediction, e.g. energy
- Node level predictions, e.g. charges
- Node level derivatives, e.g. forces
- Edge level predictions, e.g. LJ params

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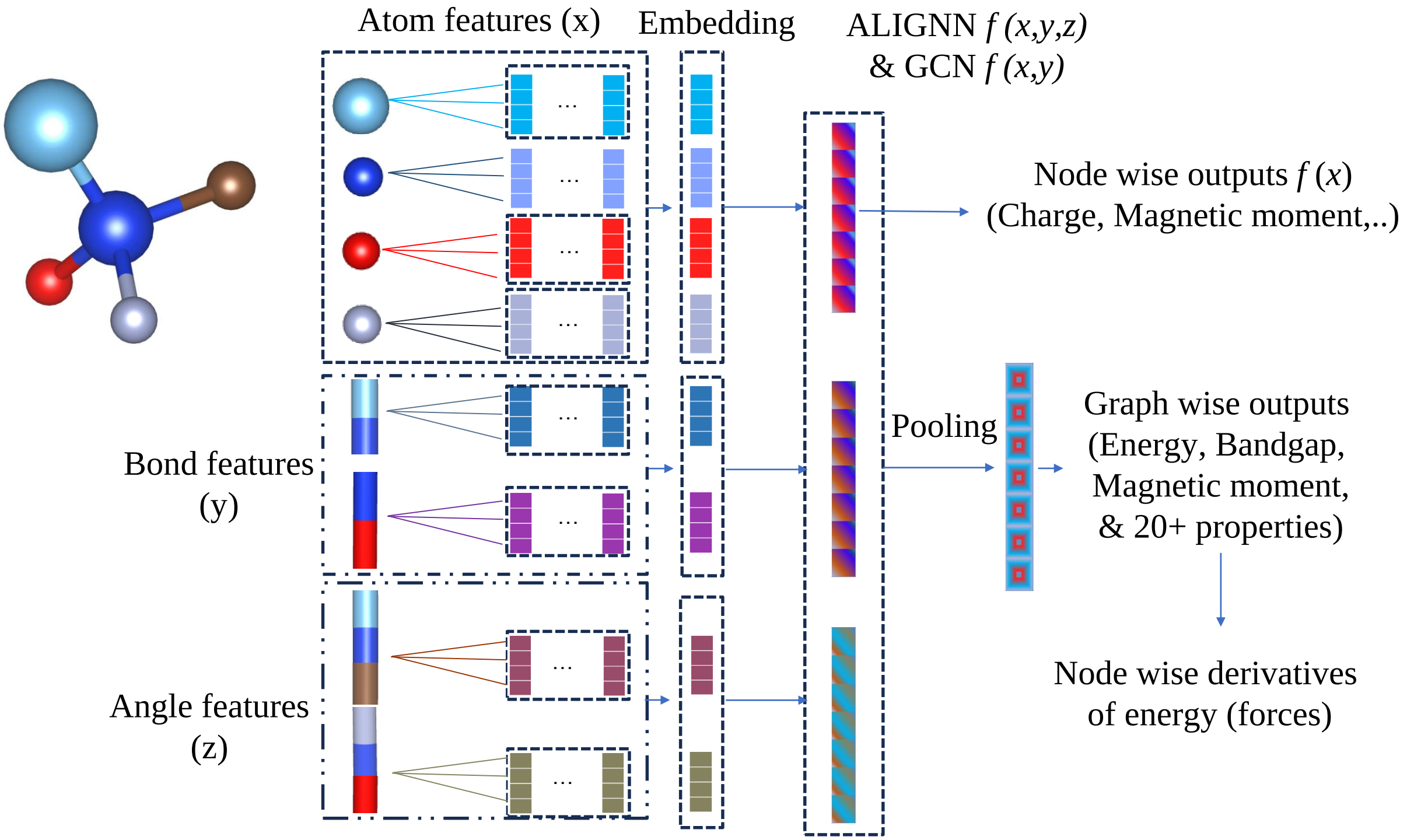

Atom features (x)
Embedding
ALIGNN $f(x,y,z)$
& GCN $f(x,y)$
Node wise outputs $f(x)$
(Charge, Magnetic moment,..)
Bond features
(y)
Pooling
Graph wise outputs
(Energy, Bandgap,
Magnetic moment,
& 20+ properties)
Angle features
(z)
Node wise derivatives
of energy (forces)

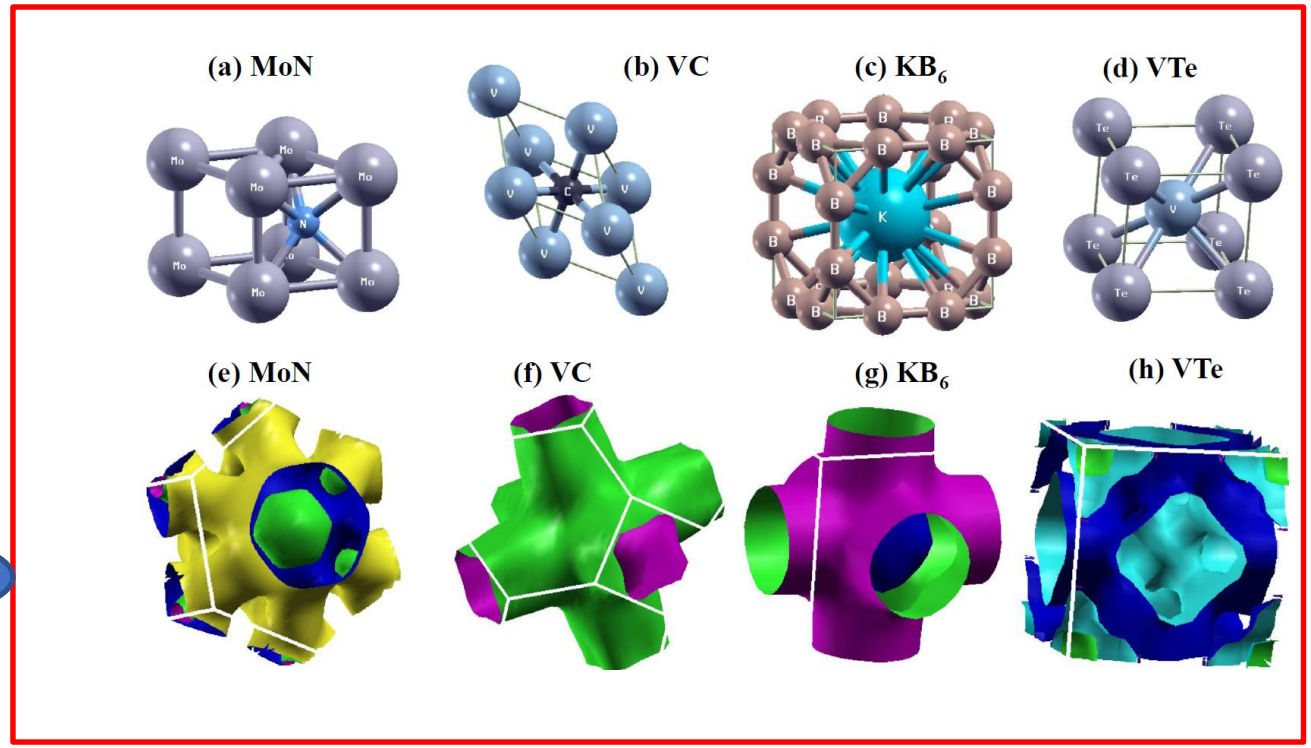
Performance on the JARVIS-DFT Dataset

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
ϵ_x (OPT)	No unit	57.40	24.83	27.17	20.40	2.81
ϵ_y (OPT)	No unit	57.54	25.03	26.62	19.99	2.88
ϵ_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

BCS Superconductors



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Article | Open access | Published: 22 November 2022

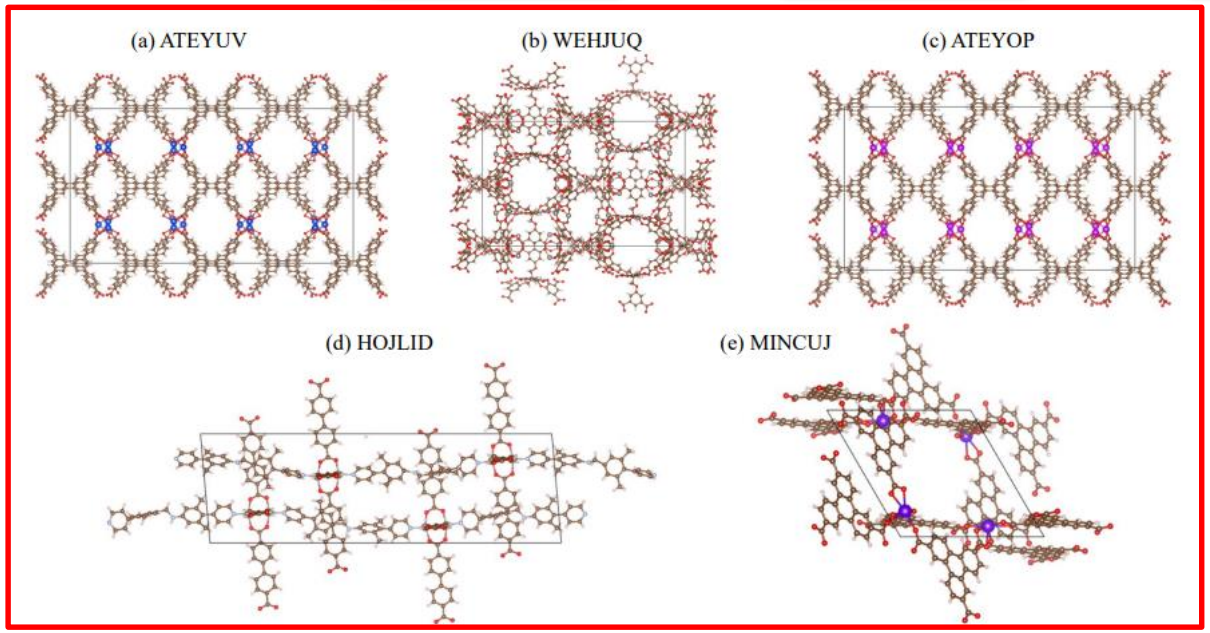
Designing high-T_C superconductors with BCS-inspired screening, density functional theory, and deep-learning

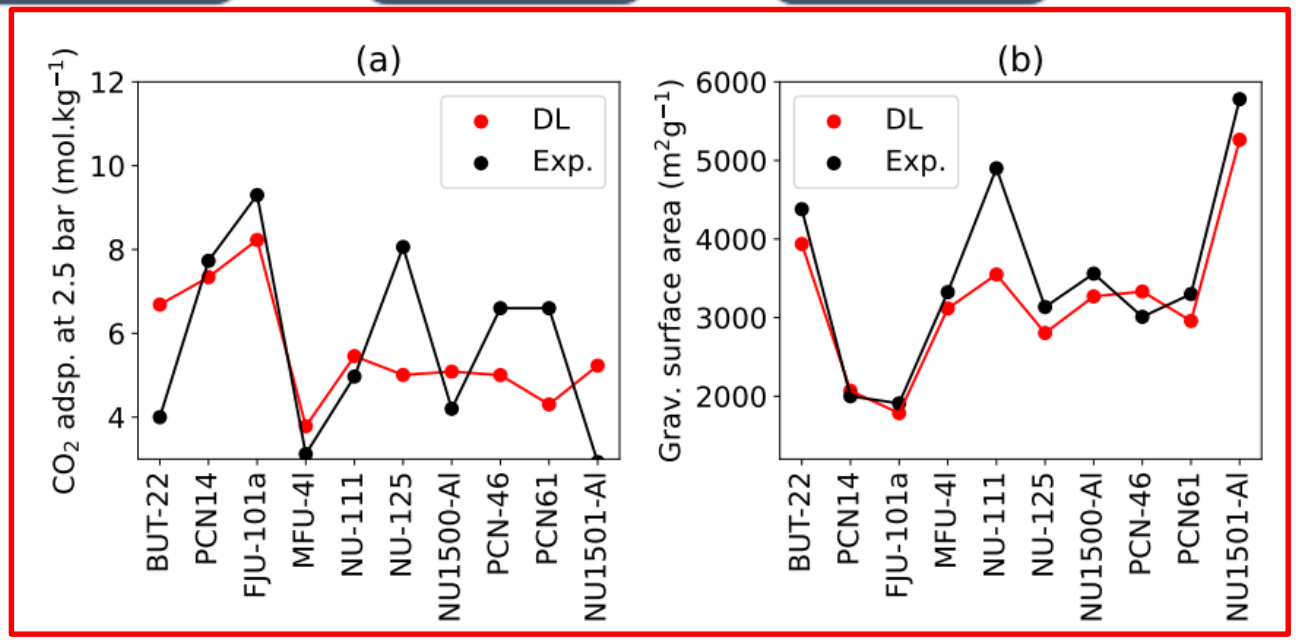
Kamal Choudhary & Kevin Garrity

- 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

CO_2 capture & MOFs

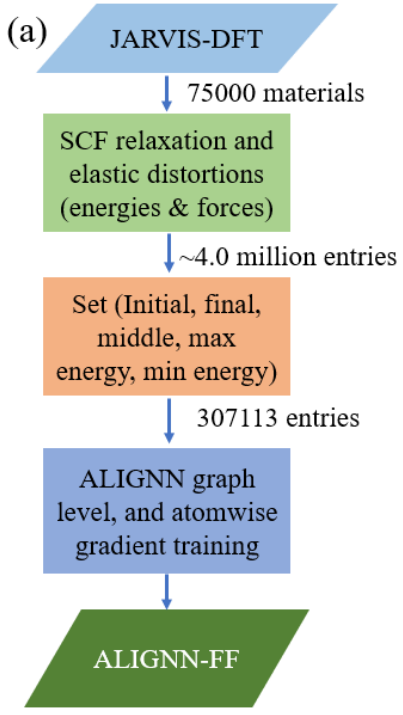
DL model for predicting CO_2 adsorption in MOFs (using hMOF GCMC data)

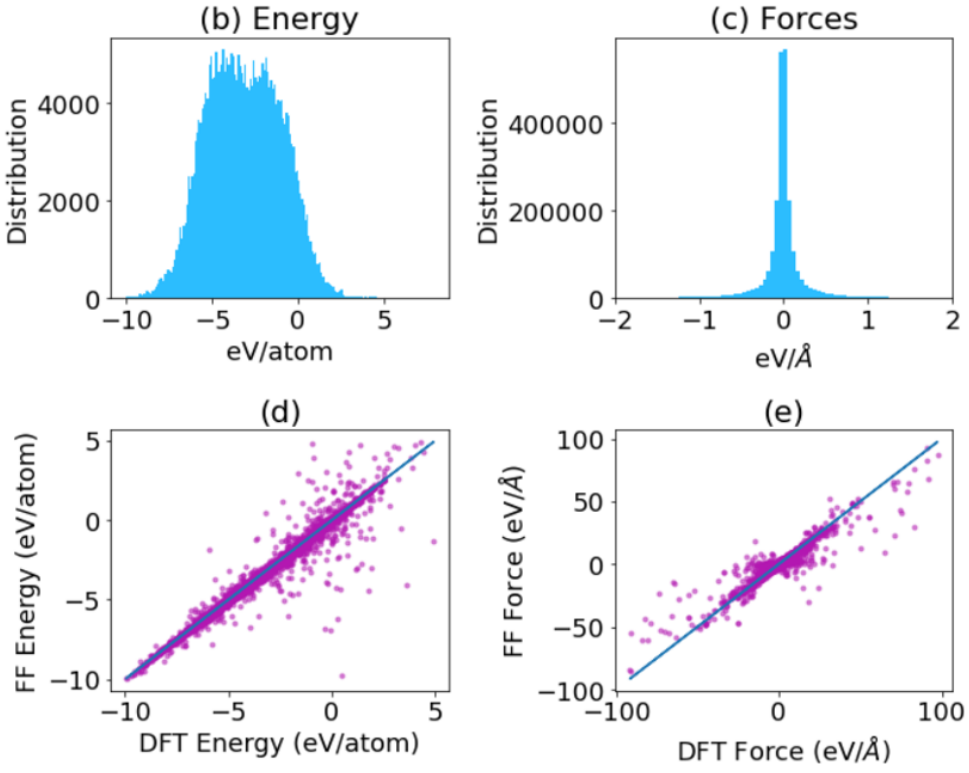




Choudhary et al., Computational Materials Science 210, 111388 (2022)

Unified GNN Force-field





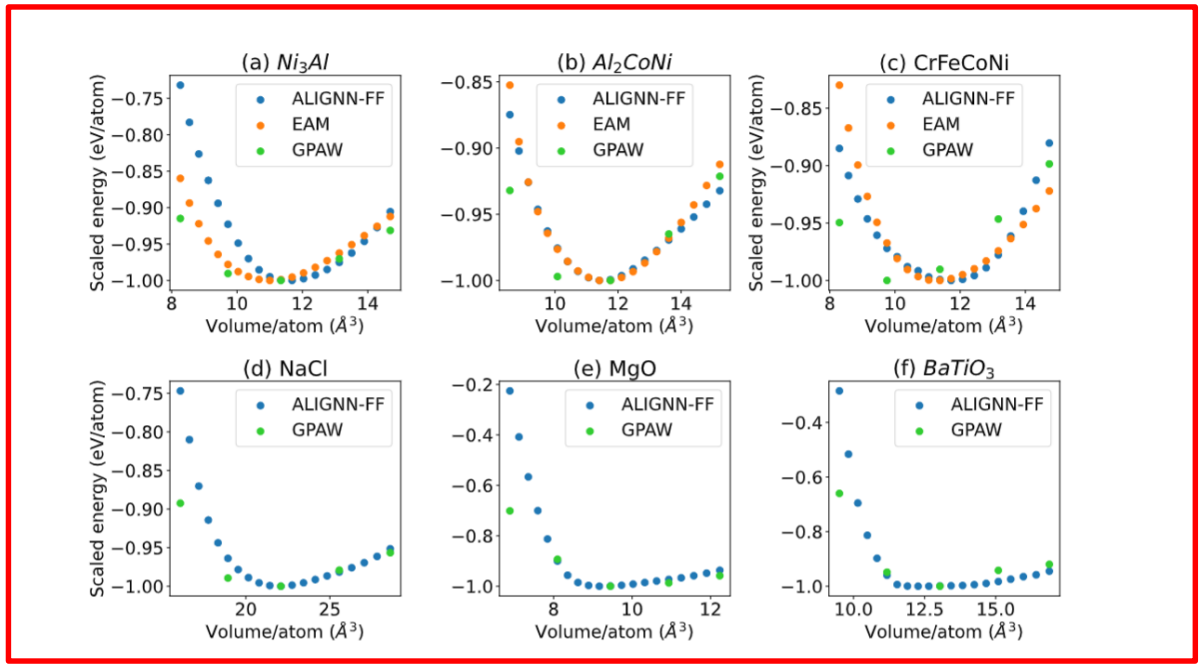
Weight	MAE-Energies (eV/atom)	MAE-Forces (eV/Å)
0.1	0.034	0.092
0.5	0.044	0.089
1.0	0.051	0.088
5.0	0.082	0.054
10.0	0.086	0.047

- Simulate any combination of 89 elements from the periodic table
- Structure optimization & Phonon property predictions

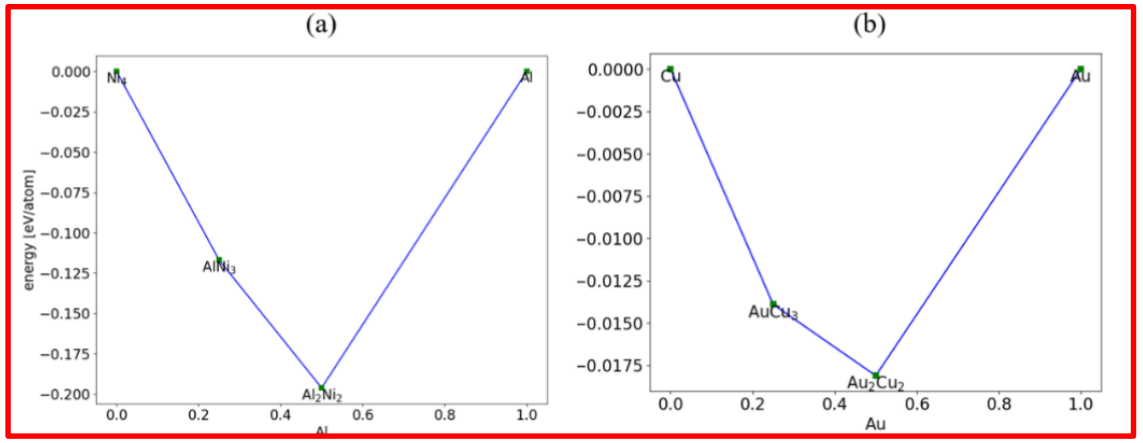
Examples

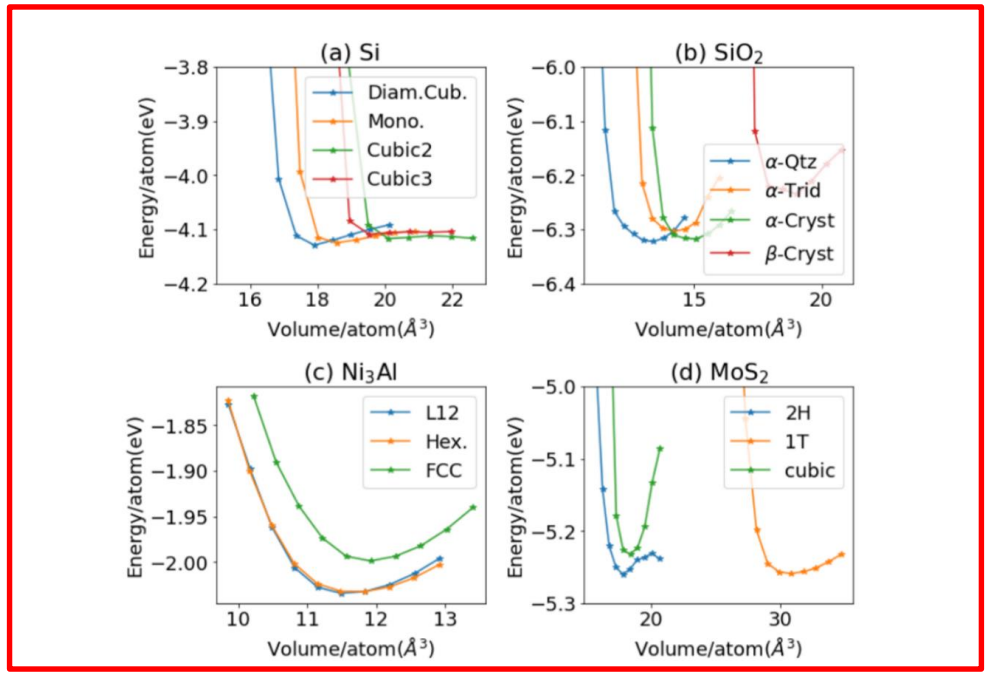
Notebooks	Google Colab	Descriptions
Regression model	Open in Colab	Examples for developing single output regression model for exfoliation energies of 2D materials.
MLFF	Open in Colab	Examples of training a machine learning force field for Silicon.
ALIGNN-FF Relaxer+EV_curve+Phonons+Interface gamma_surface+Interface separation	Open in Colab	Examples of using pre-trained ALIGNN-FF force-field model.
Miscellaneous tasks	Open in Colab	Examples for developing single output (such as formation energy, bandgaps) or multi-output (such as phonon DOS, electron DOS) Regression or Classification (such as metal vs non-metal), Using several pretrained models.

Unified GNN Force-field



Genetic algorithm





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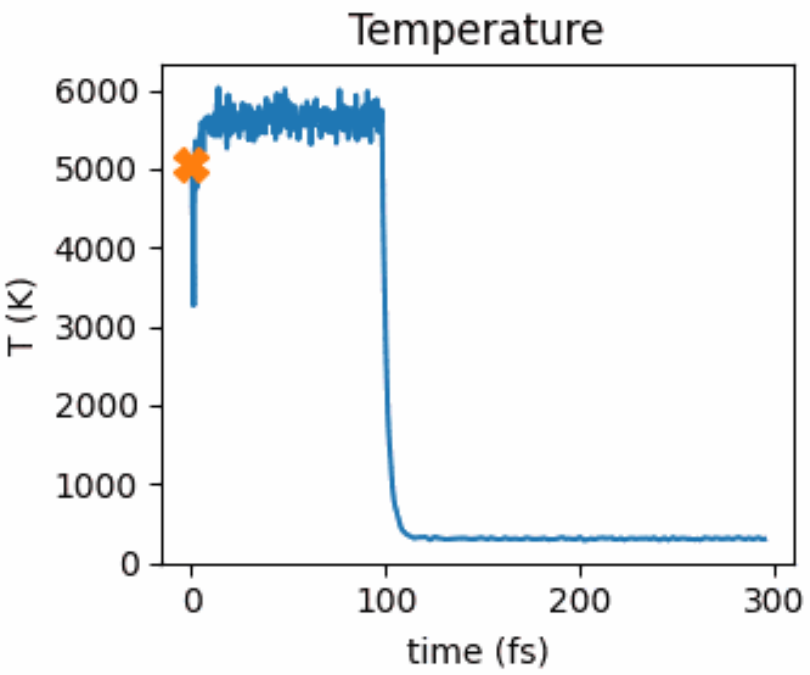
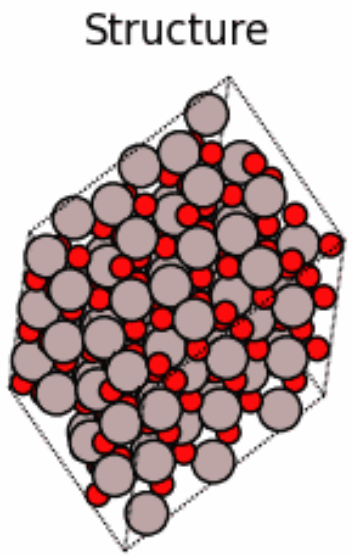
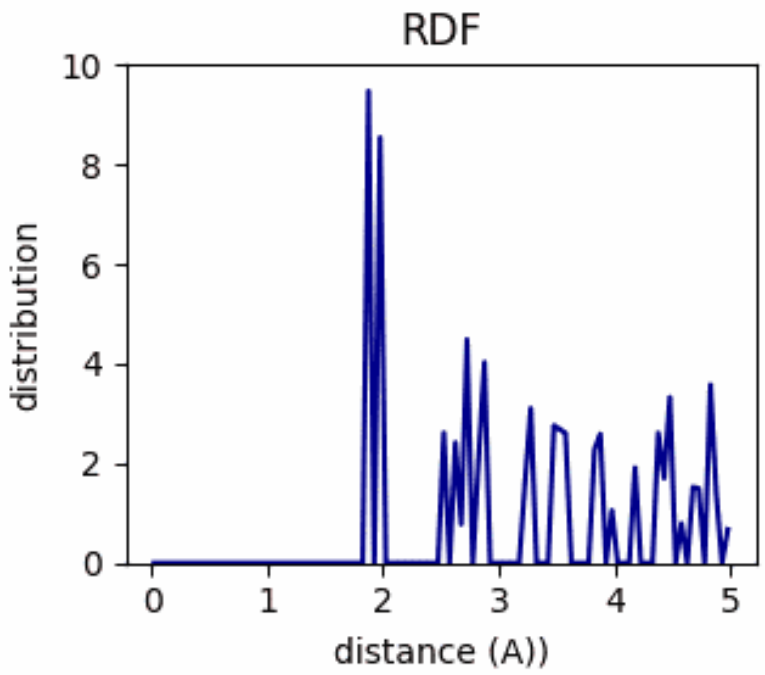
Unified graph neural network force-field for the periodic table: solid state applications

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

Al_2O_3 Melt-Quench Simulation Example

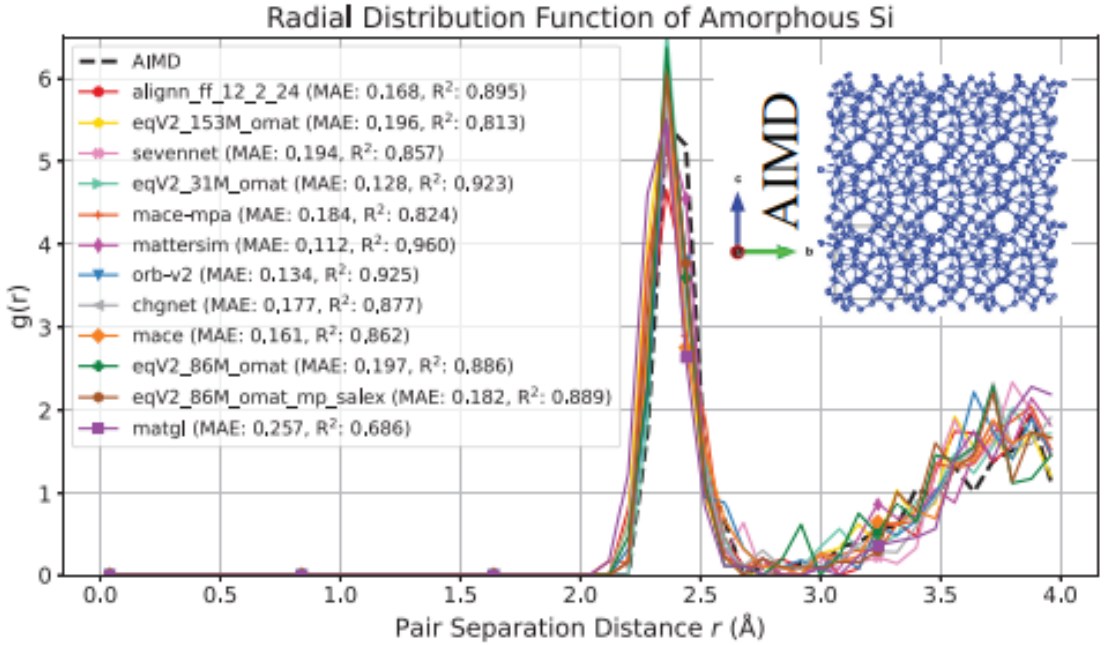






CHIPS-FF

uMLFF Type	err_a Å	err_b Å	err_c Å	err_vol Å^3	err_kv GPa	err_c11 GPa	err_c44 GPa	err_phonon cm^{-1}	Time seconds
alignn_ff	0.087	0.102	0.137	9.95	122	196	74	150	8.8 x 10^4
chgnet	0.046	0.049	0.109	3.58	85	59	45	68	3.5 x 10^4
eqV2_153M_omat	0.036	0.040	0.111	2.90	117	70	32	49	1.6 x 10^2
eqV2_31M_omat	0.029	0.032	0.099	3.05	115	78	37	48	3.4 x 10^5
eqV2_31M_omat_mp_salex	0.028	0.030	0.096	3.17	112	47	41	48	2.7 x 10^5
eqV2_86M_omat	0.033	0.040	0.094	3.41	116	85	35	49	9.7 x 10^5
eqV2_86M_omat_mp_salex	0.027	0.030	0.100	3.14	114	45	35	48	7.2 x 10^5
mace	0.035	0.038	0.084	3.00	94	43	38	58	7.2 x 10^4
mace-alexandria	0.081	0.086	0.206	6.05	76	96	45	81	2.5 x 10^5
mace-mpa	0.044	0.046	0.098	3.57	110	35	34	49	8.4 x 10^4
matgl	0.052	0.057	0.128	3.50	83	64	41	78	1.7 x 10^4
matgl-direct	0.044	0.046	0.106	2.88	84	73	50	85	2.5 x 10^4
mattersim	0.031	0.033	0.110	3.18	110	32	32	48	5.9 x 10^4
orb-d3-v2	0.031	0.030	0.048	1.90	130	74	74	52	2.7 x 10^4
orb-v2	0.023	0.025	0.159	3.38	119	80	74	49	2.4 x 10^4
sevennet	0.035	0.038	0.100	3.43	103	46	37	53	5.7 x 10^4



arXiv > cond-mat > arXiv:2412.10516

Condensed Matter > Materials Science

[Submitted on 13 Dec 2024 (v1), last revised 15 Jan 2025 (this version, v3)]

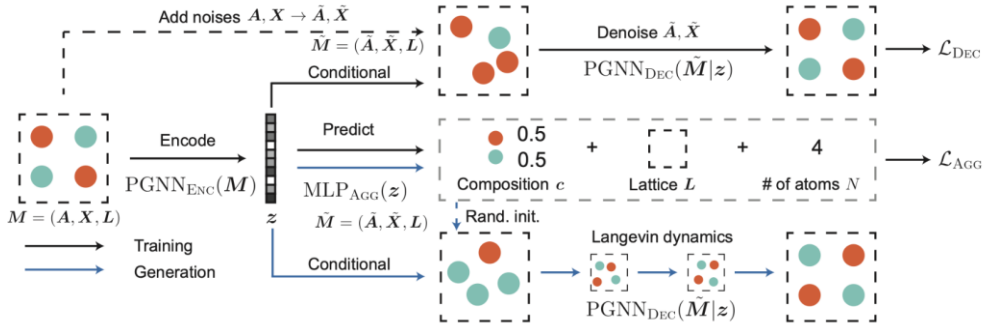
CHIPS-FF: Evaluating Universal Machine Learning Force Fields for Material Properties

Daniel Wines, Kamal Choudhary

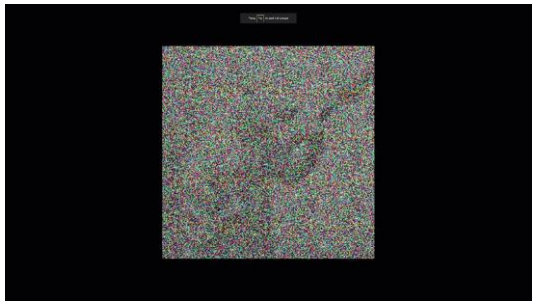
https://arxiv.org/abs/2412.10516

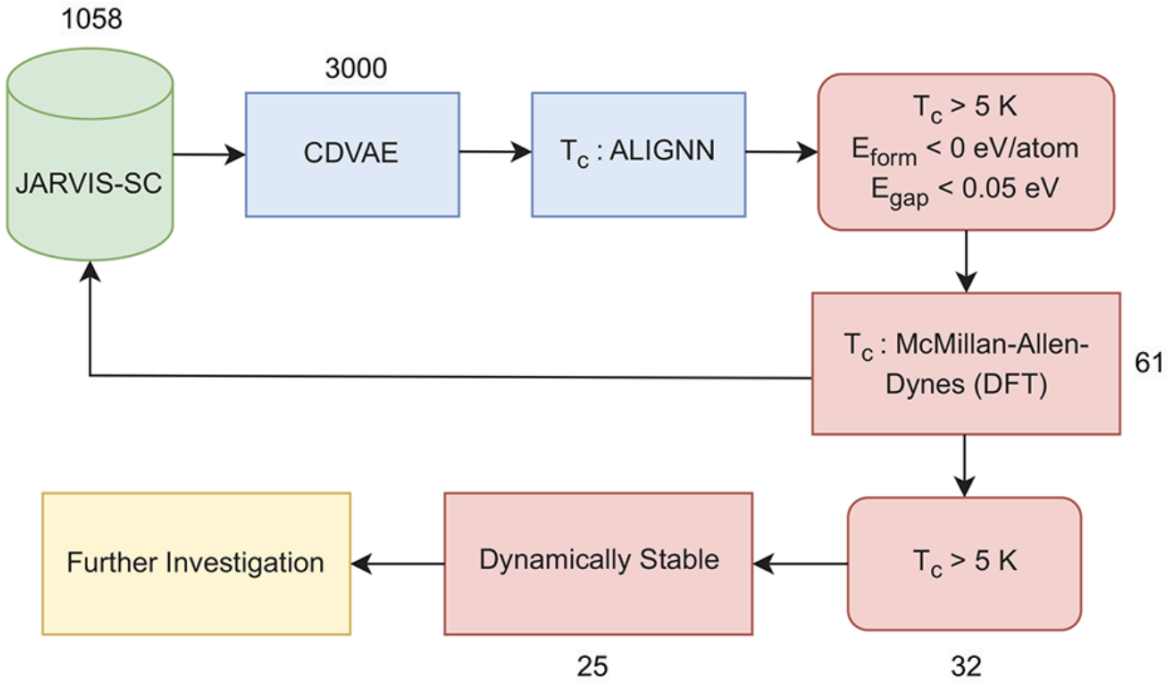
Inverse Design (superconductors)

- Crystal diffusion variational autoencoder (CDVAE) for inverse design
- Trained on JARVIS-SC data
- Properties screened with ALIGNN, verified with DFT

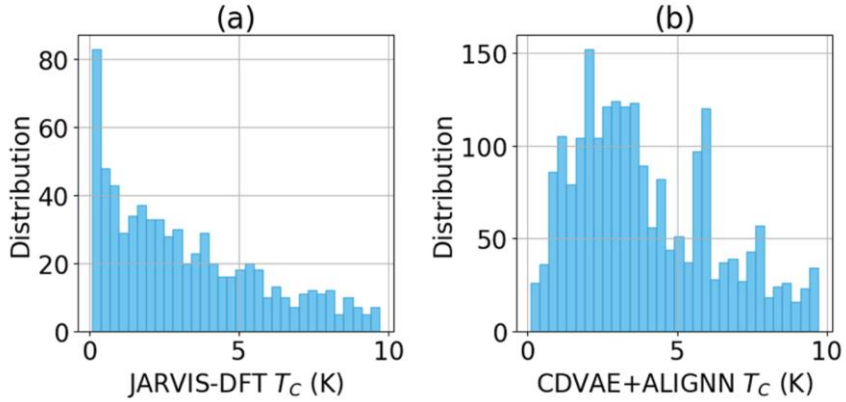


Xie et al. arXiv:2110.06197 (2022)

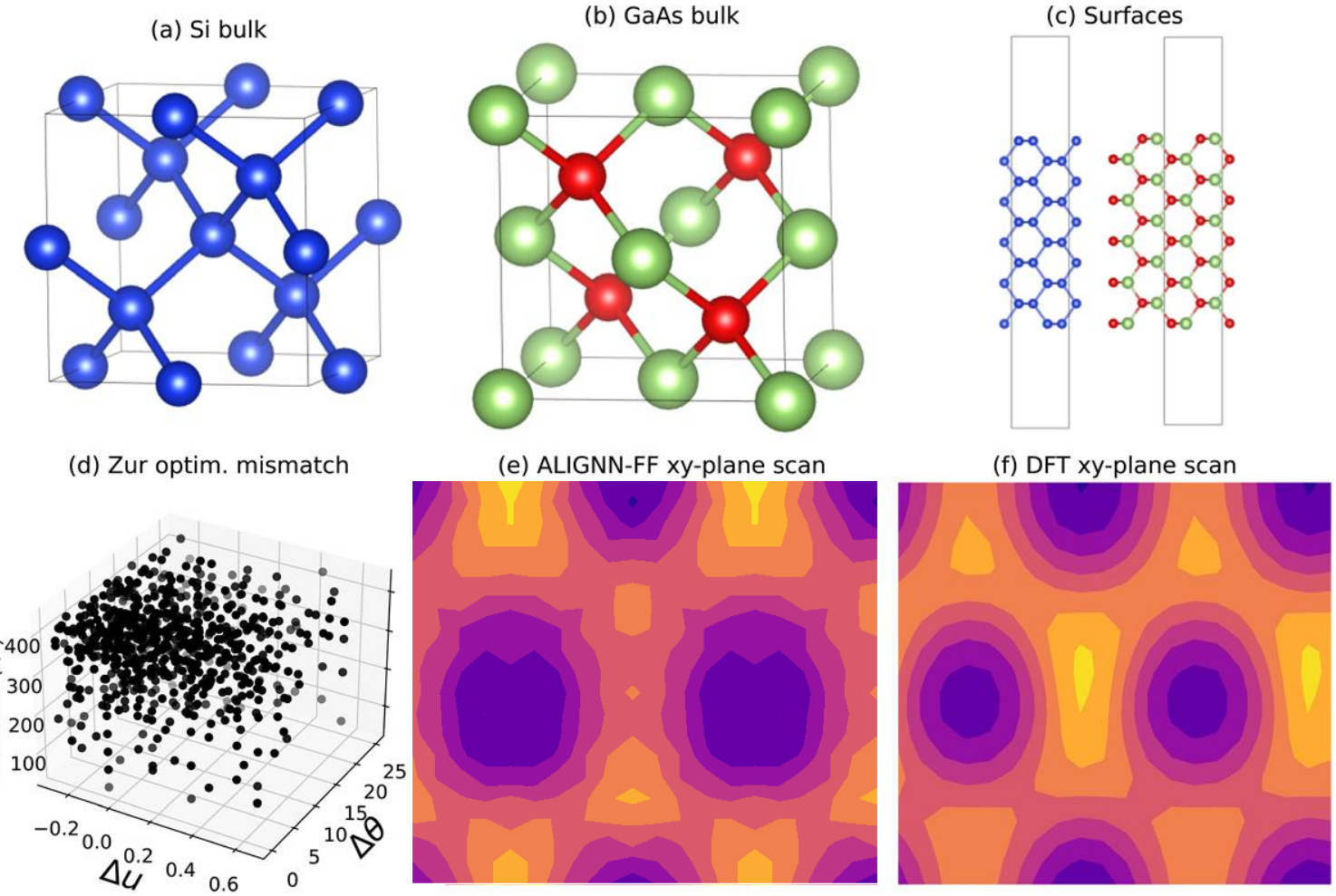




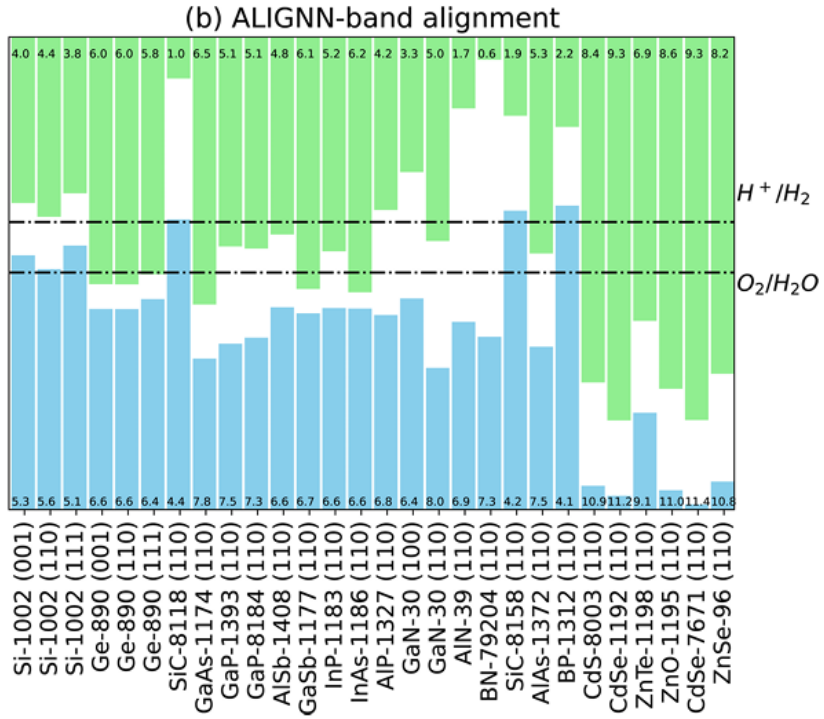
Wines, Xie, Choudhary, J. Phys. Chem. Lett., 14, 6630-6638 (2023)



InterMat: Interface Materials Design (Semicons)

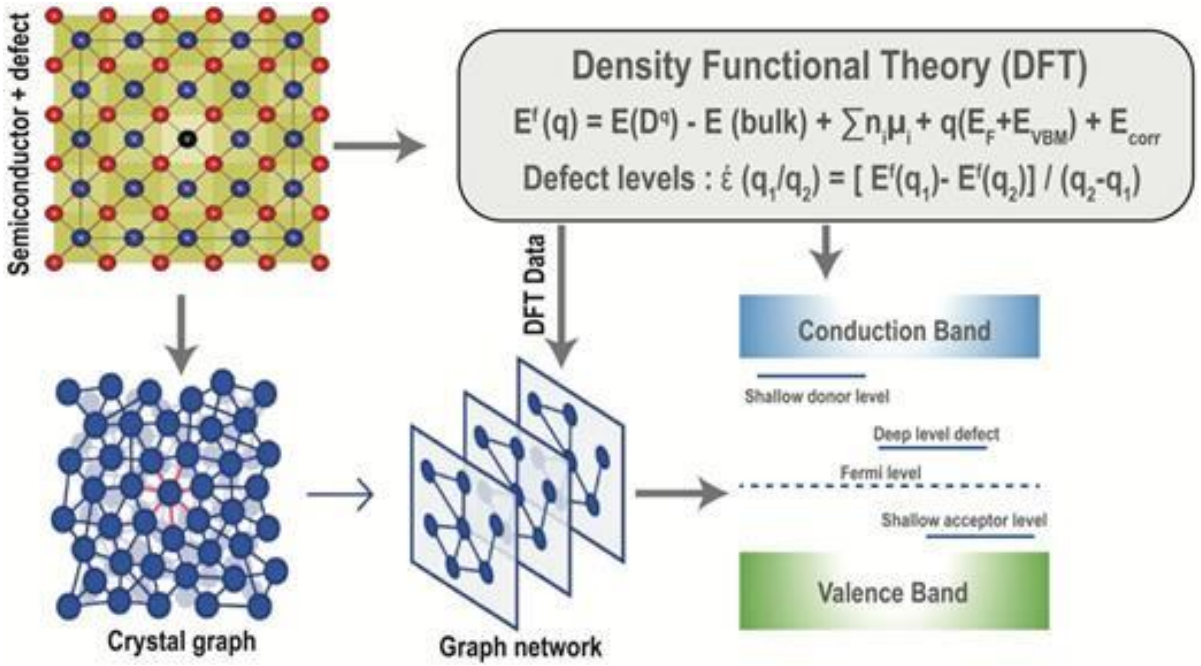


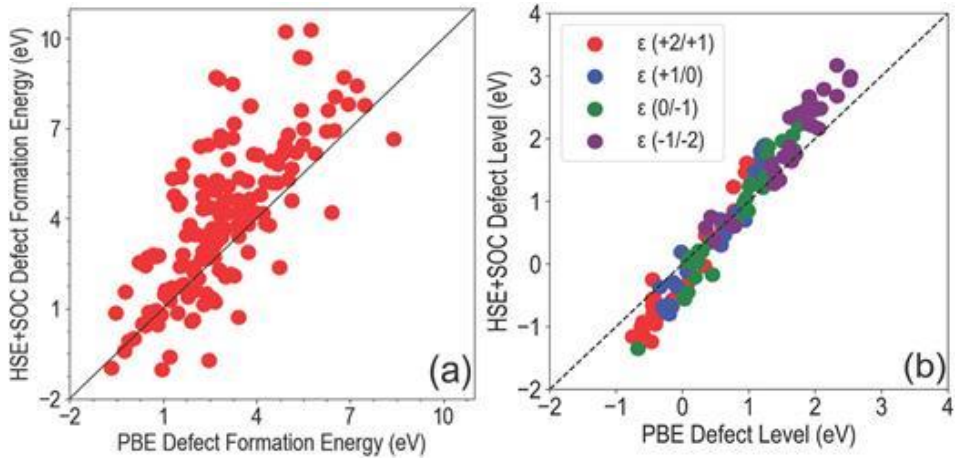
- ALIGNN+DFT for accelerated interface design
- Benchmarked band-offset predictions
- General workflow for materials design



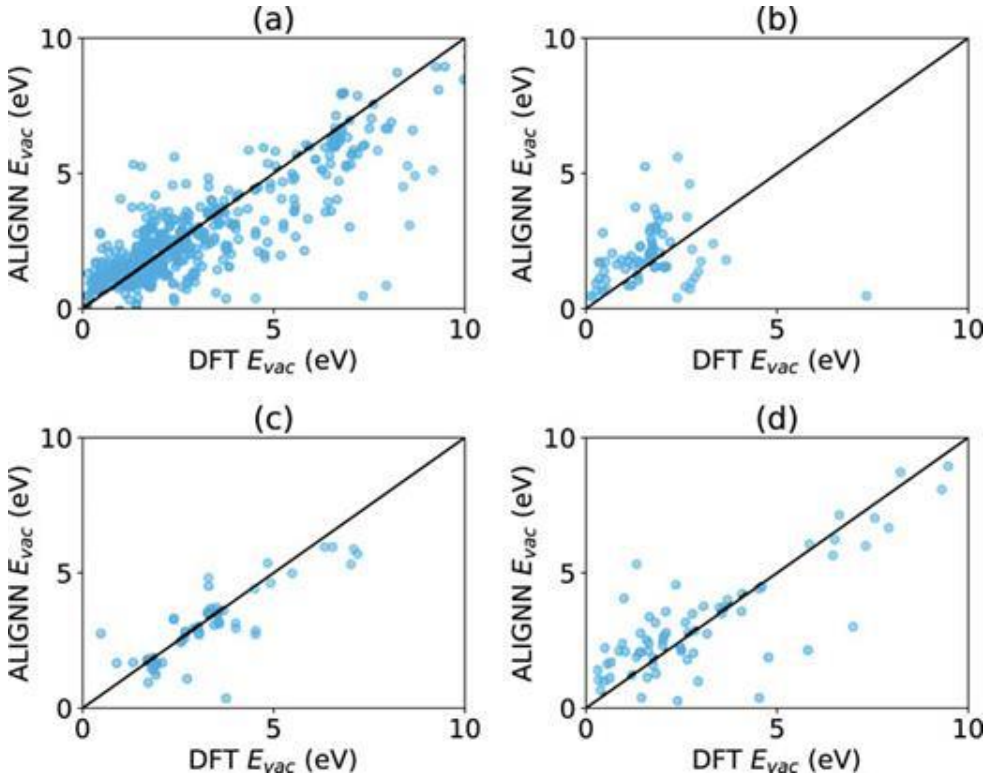
DOI: 10.1039/D4DD00031E Digital Discovery, 2024

DefectMat: Defect Materials Design



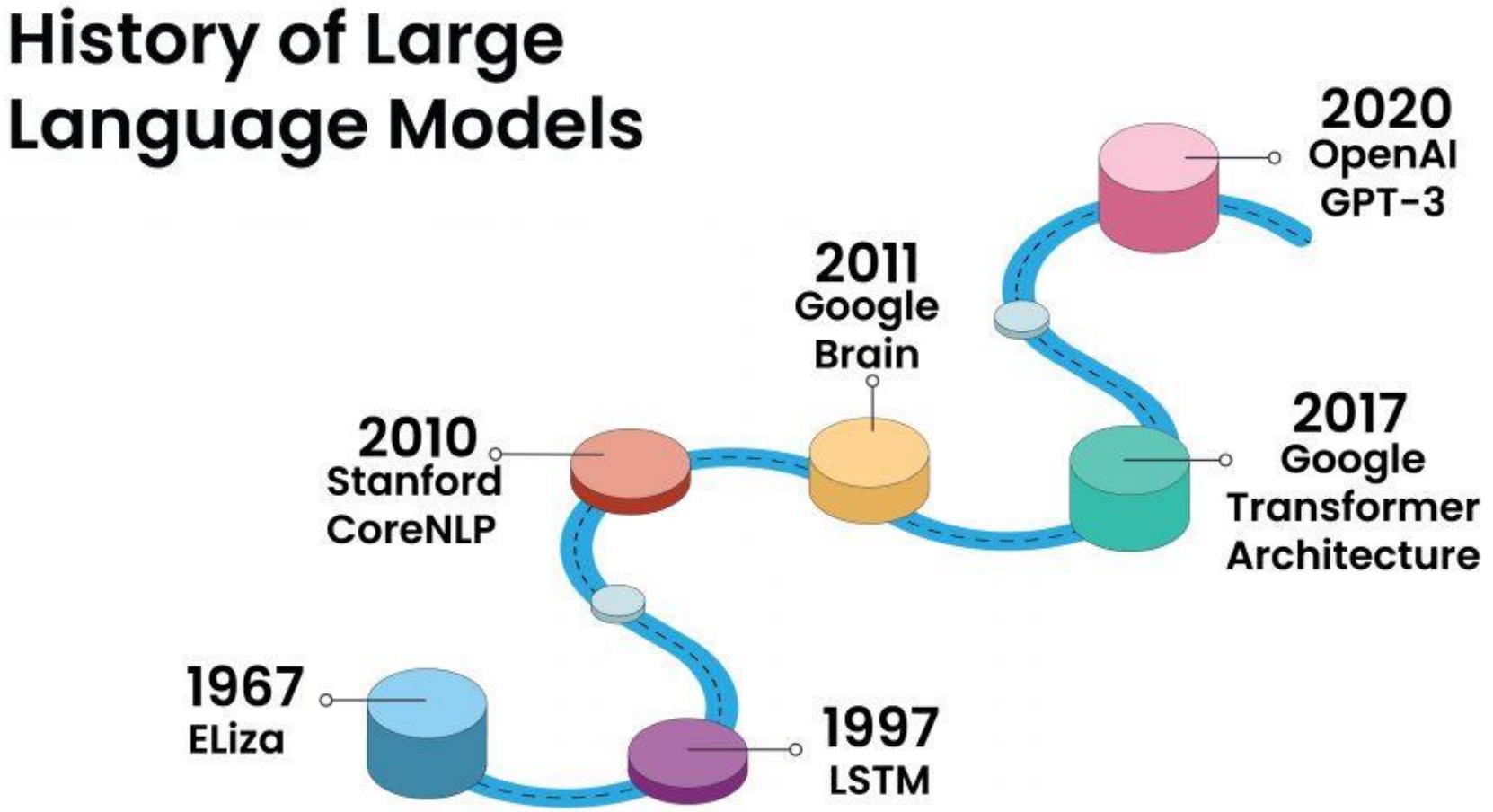


- ALIGNN+DFT for accelerated defect design
- Benchmarked vacancy formation predictions
- Neutral and charged defects



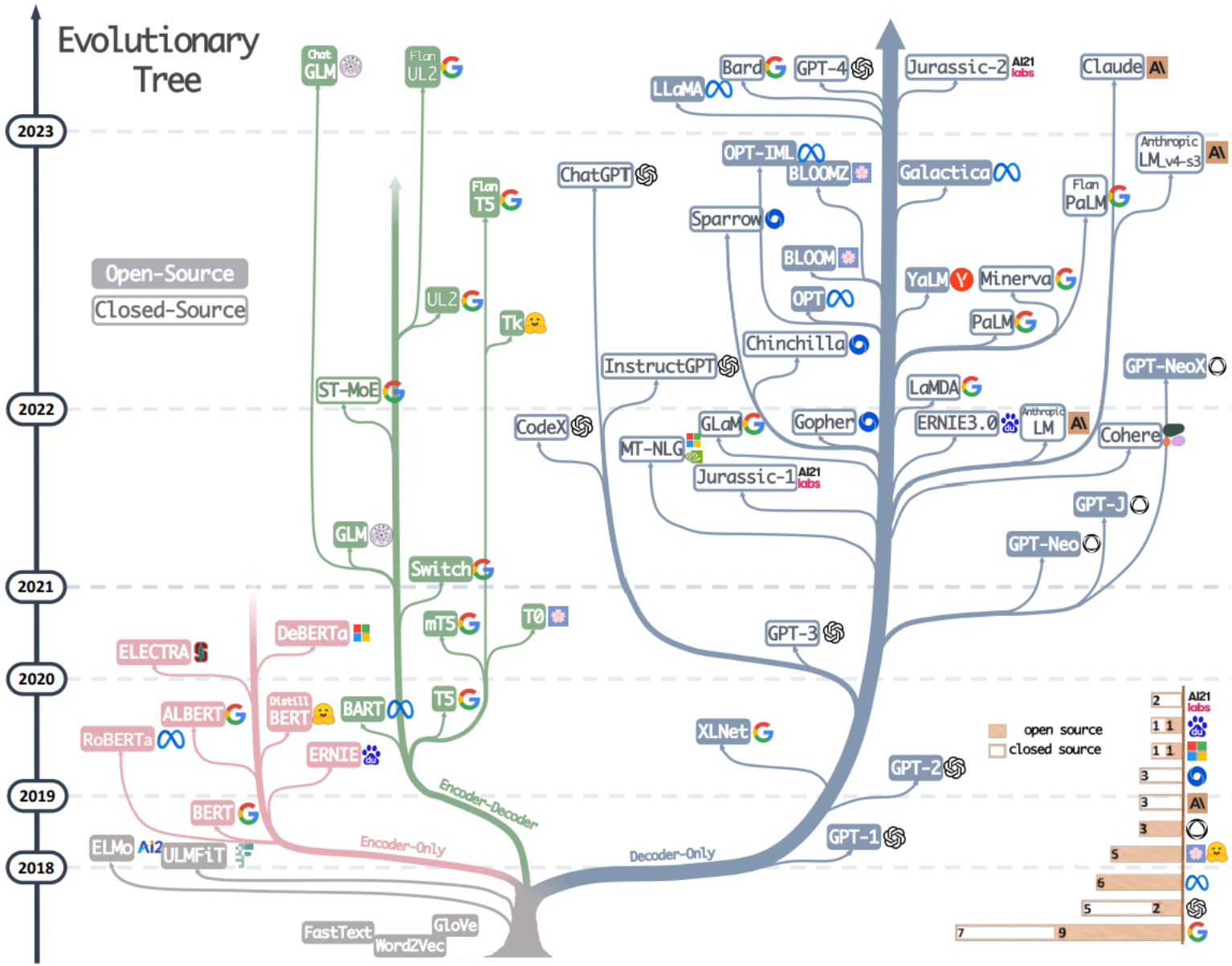
AIP Advances 2023, APL Machine Learning 2024

Large Language Models



https://www.scribbledata.io/blog/large-language-models-history-evolutions-and-future/

LLM Evolution



https://arxiv.org/pdf/2304.13712

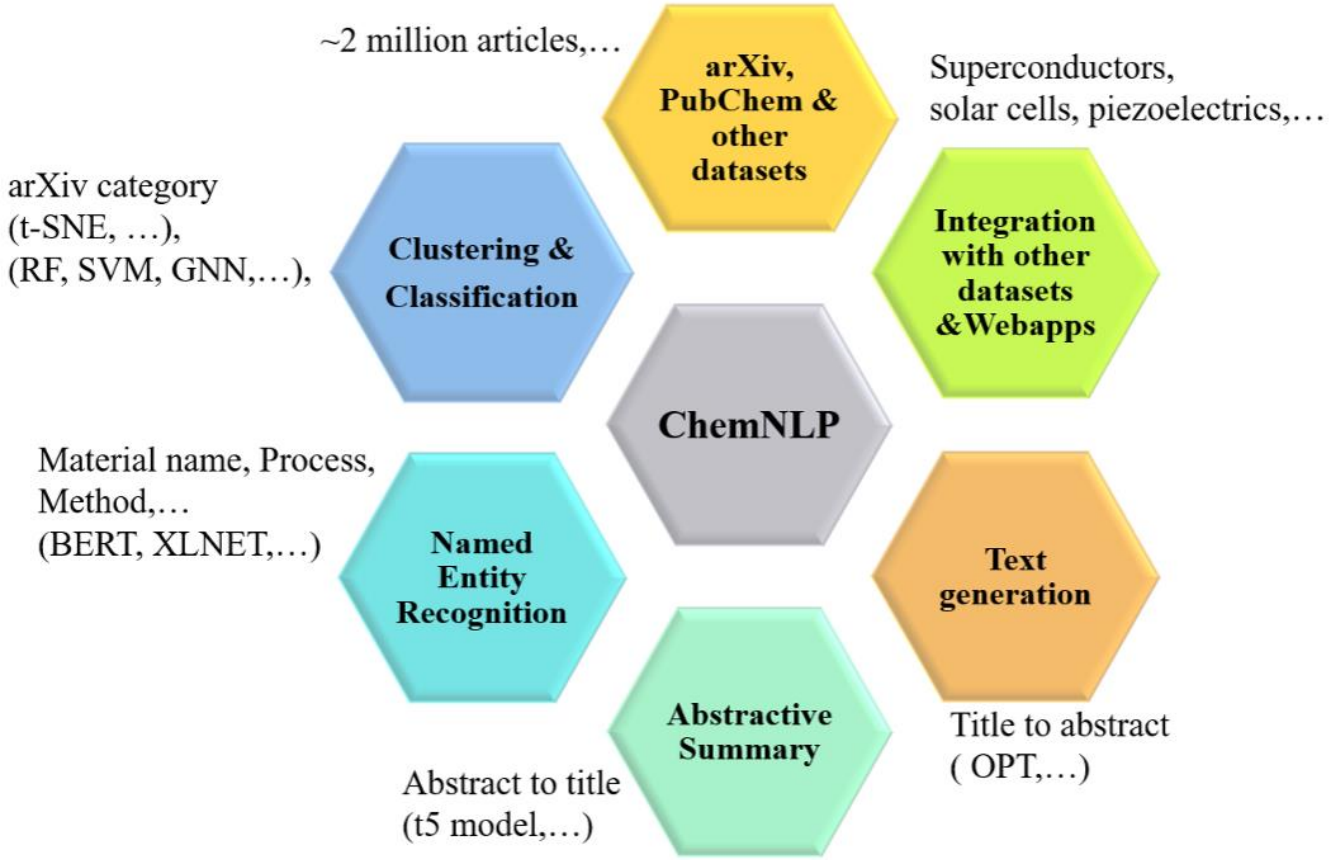
LLM Applications for MSE

DOI: 10.1039/D3DD00113J (Perspective) *Digital Discovery*, 2023, **2**, 1233-1250

14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon†

Kevin Maik Jablonka *[a], **Qianxiang Ai**‡ [b], **Alexander Al-Feghali**‡ [c], **Shruti Badhwar**‡ [d], **Joshua D. Bocarsly**‡ [e], **Andres M. Bran**‡ [fg], **Stefan Bringuier**‡ [h], **L. Catherine Brinson**‡ [i], **Kamal Choudhary**‡ [j], **Defne Circi**‡ [i], **Sam Cox**‡ [k], **Wibe A. de Jong**‡ [l], **Matthew L. Evans**‡ [mn], **Nicolas Gastellu**‡ [c], **Jerome Genzling**‡ [c], **María Victoria Gil**‡ [o], **Ankur K. Gupta**‡ [l], **Zhi Hong**‡ [p], **Alishba Imran**‡ [q], **Sabine Kruschwitz**‡ [r], **Anne Labarre**‡ [c], **Jakub Lála**‡ [s], **Tao Liu**‡ [c], **Steven Ma**‡ [c], **Sauradeep Majumdar**‡ [a], **Garrett W. Merz**‡ [t], **Nicolas Moitessier**‡ [c], **Elias Moubarak**‡ [a], **Beatriz Mouriño**‡ [a], **Brenden Pelkie**‡ [u], **Michael Pieler**‡ [vw], **Mayk Caldas Ramos**‡ [k], **Bojana Ranković**‡ [fg], **Samuel G. Rodriques**‡ [s], **Jacob N. Sanders**‡ [x], **Philippe Schwaller**‡ [fg], **Marcus Schwarting**‡ [y], **Jiale Shi**‡ [b], **Berend Smit**‡ [a], **Ben E. Smith**‡ [e], **Joren Van Herck**‡ [a], **Christoph Völker**‡ [r], **Logan Ward**‡ [z], **Sean Warren**‡ [c], **Benjamin Weiser**‡ [c], **Sylvester Zhang**‡ [c], **Xiaoqi Zhang**‡ [a], **Ghezal Ahmad Zia**‡ [r], **Aristana Scourtas** [aa], **K. J. Schmidt** [aa], **Ian Foster** [ab], **Andrew D. White** [k] **and Ben Blaiszik** *[aa]

ChemNLP



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C: PHYSICAL PROPERTIES OF MATERIALS AND INTERFACES | August 25, 2023

ChemNLP: A Natural Language-Processing-Based Library for Materials Chemistry Text Data

Kamal Choudhary*, and Mathew L. Kelley

Open PDF open URL

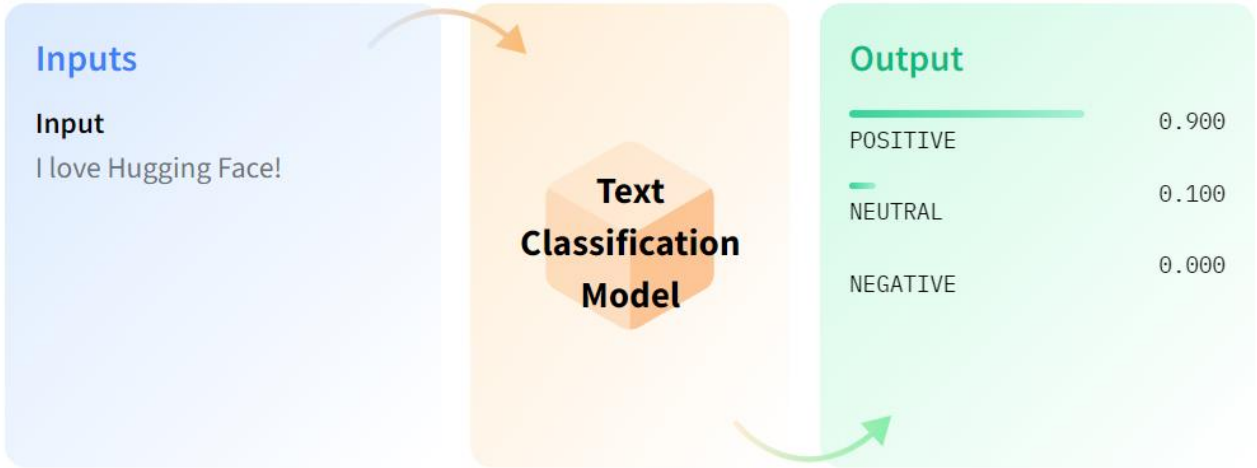
Text classification & Token classification

huggingface.co/tasks/text-classification

Tasks

Text Classification

Text Classification is the task of assigning a label or class to a given text. Some use cases are sentiment analysis, natural language inference, and assessing grammatical correctness.

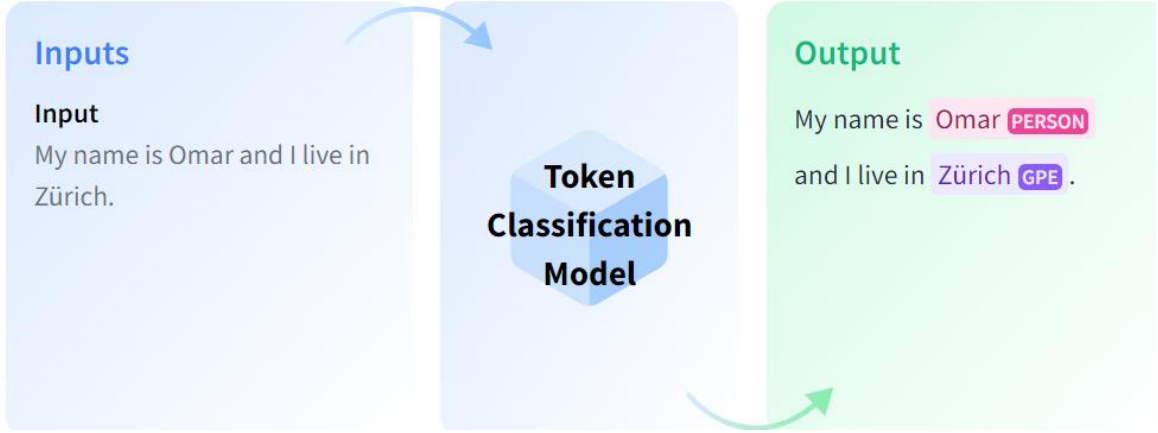


huggingface.co/tasks/token-classification

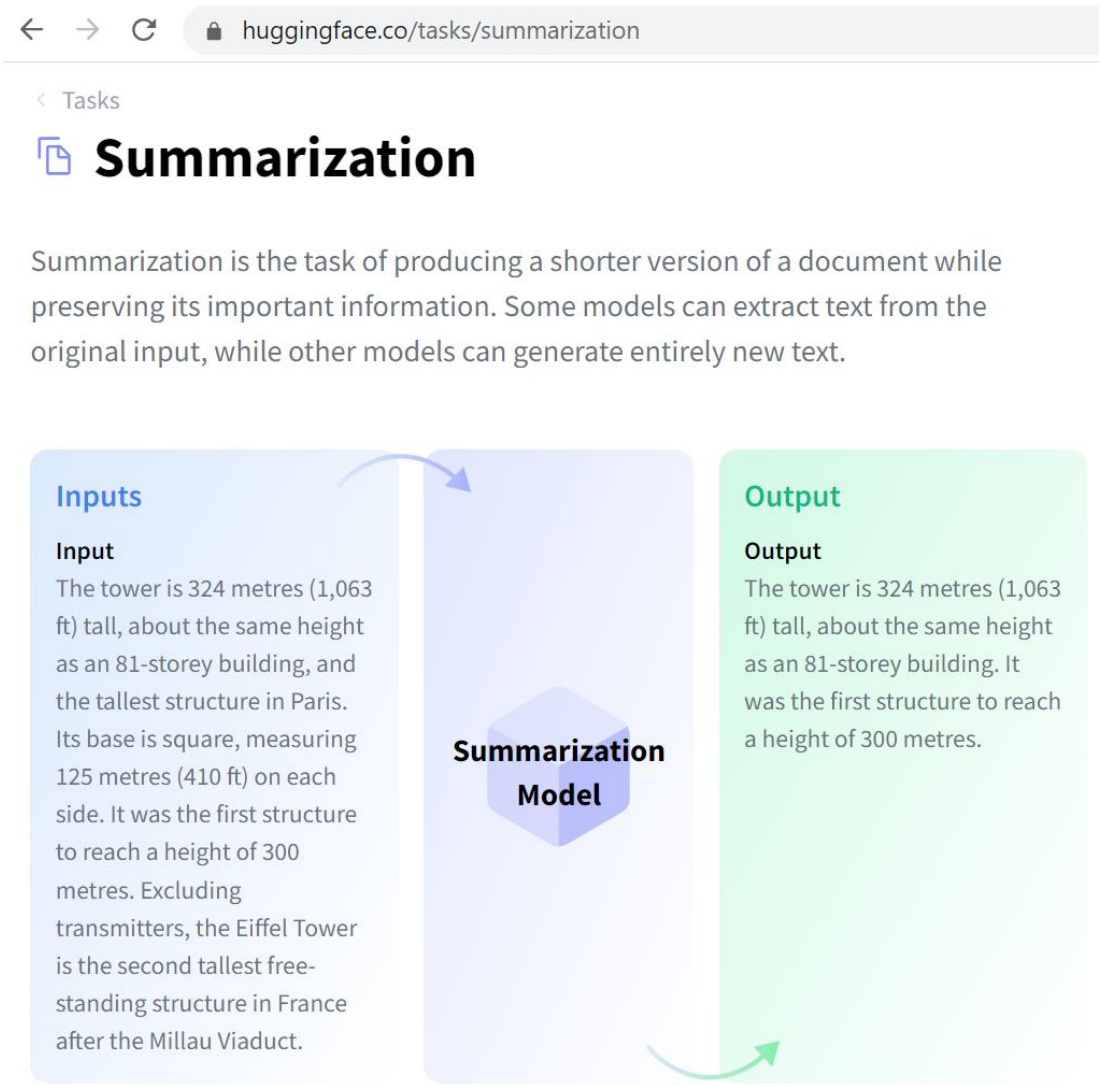
Tasks

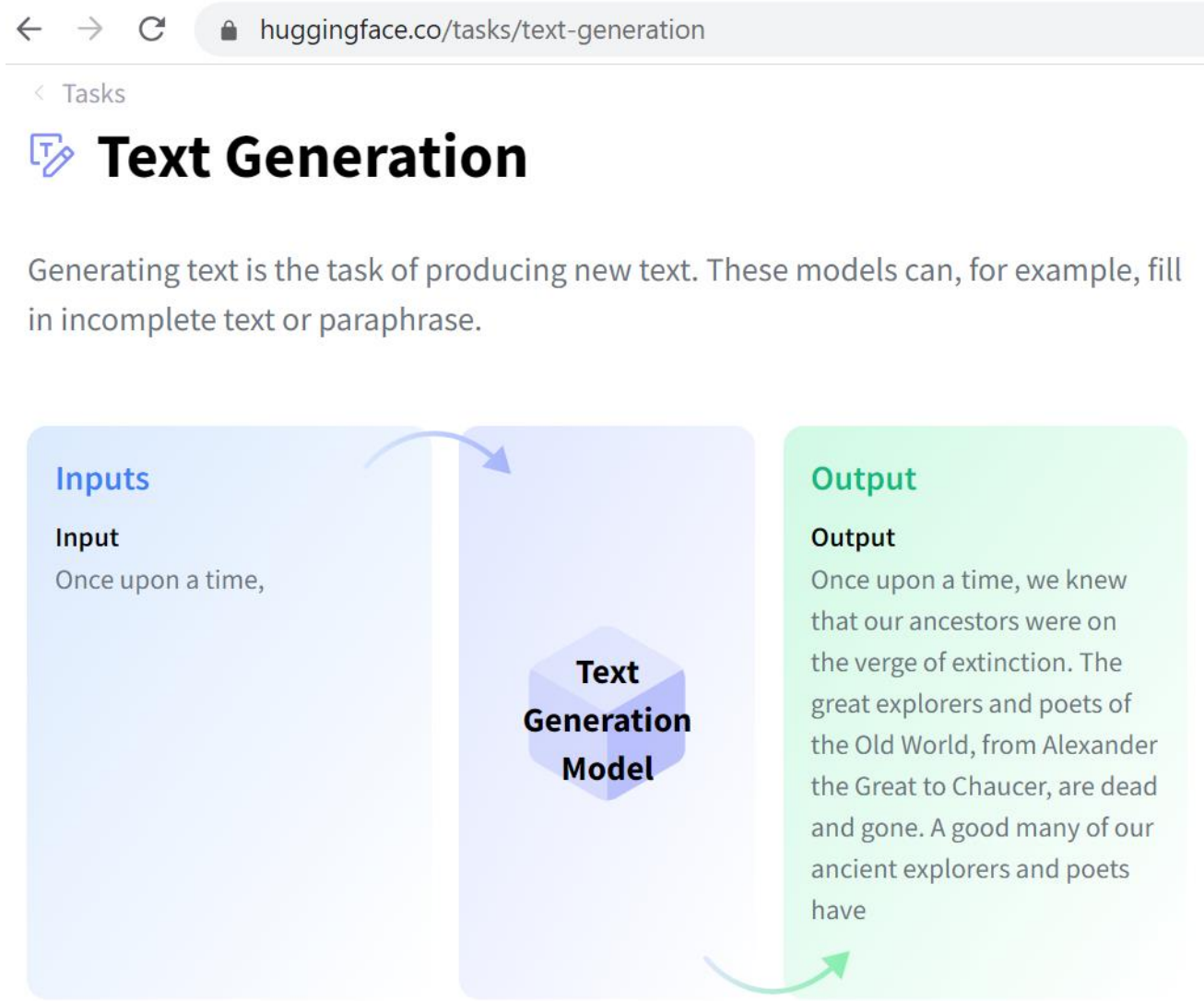
Token Classification

Token classification is a natural language understanding task in which a label is assigned to some tokens in a text. Some popular token classification subtasks are Named Entity Recognition (NER) and Part-of-Speech (PoS) tagging. NER models could be trained to identify specific entities in a text, such as dates, individuals and places; and PoS tagging would identify, for example, which words in a text are verbs nouns, and punctuation marks.

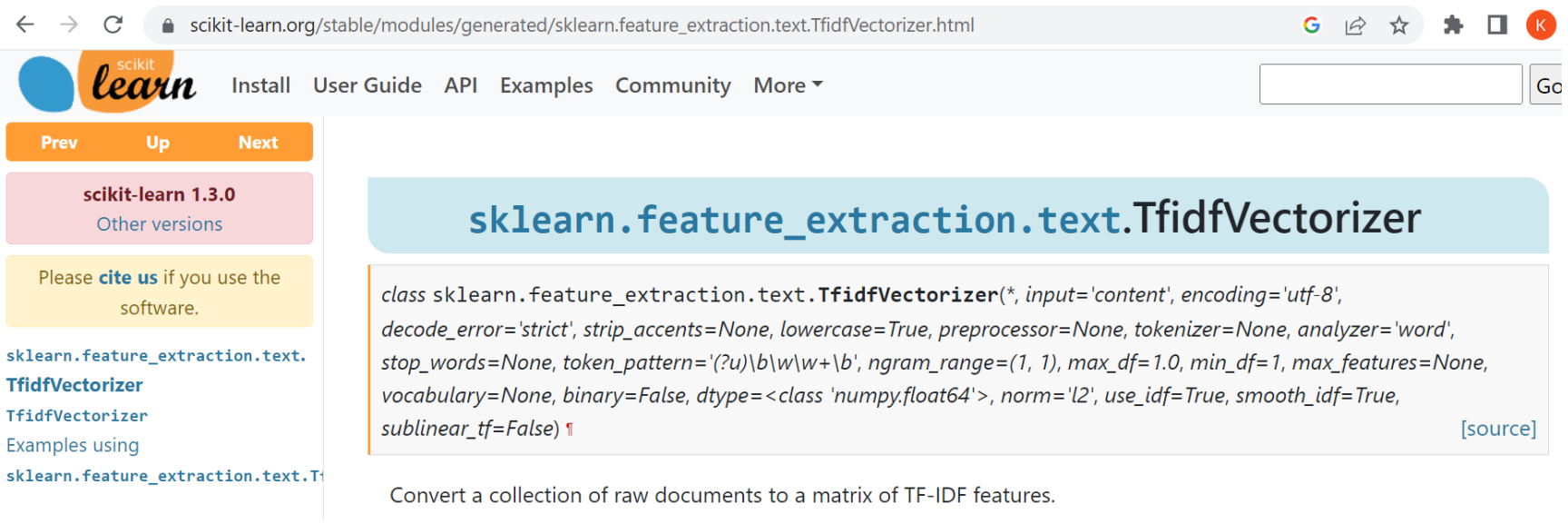


Text summarization & Text-generation





Conventional NLP: TFIDF



$$TFIDF\ score\ for\ term\ i\ in\ document\ j = TF(i,j) * IDF(i)$$

where

$IDF = Inverse\ Document\ Frequency$

$TF = Term\ Frequency$

$$TF(i,j) = \frac{\text{Term i frequency in document j}}{\text{Total words in document j}}$$

$$IDF(i) = \log_2\left(\frac{\text{Total documents}}{\text{documents with term i}}\right)$$

and

$t = Term$

$j = Document$

In [21]:
```
sentence = "The oldest human fossil is the skull discovered in the Cave of Aroeira in Almonda."

TfidfVec = TfidfVectorizer()
tfidf = TfidfVec.fit_transform([sentence])

cols = TfidfVec.get_feature_names()
matrix = tfidf.todense()
pd.DataFrame(matrix,columns = cols,index=["Tf-Idf"])
```

Out[21]:

	almonda	aroeira	cave	discovered	fossil	human	in	is	of	oldest	skull	the
Tf-Idf	0.208514	0.208514	0.208514	0.208514	0.208514	0.208514	0.417029	0.208514	0.208514	0.208514	0.208514	0.625543

https://www.kaggle.com/code/ashoksrinivas/nlp-with-tfidf-neural-networks
https://scikit-learn.org/stable/modules/generated/sklearn.feature_extraction.text.TfidfVectorizer.html
https://i.stack.imgur.com/mtmP6.png

Conventional NLP: TFIDF

Term Frequency (TF)

TF measures how frequently a term appears in a document. It is calculated as:

$$TF(t, d) = \frac{\text{Number of times the term appears in the document}}{\text{Total number of terms in the document}}$$

Example:

If a document has 100 words and the word "coffee" appears 5 times, the TF for "coffee" would be:

$$TF_{\text{coffee}} = \frac{5}{100} = 0.05$$

Inverse Document Frequency (IDF)

IDF measures how important or unique a term is across an entire corpus. It is calculated as:

$$IDF(t, D) = \log\left(\frac{\text{Total number of documents}}{\text{Number of documents containing the term}}\right)$$

Example:

If we have 1,000 documents and the word "coffee" appears in 10 of them, the IDF for "coffee" would be:

$$IDF_{\text{coffee}} = \log\left(\frac{1000}{10}\right) = \log(100) = 2$$

Using the previous examples where:

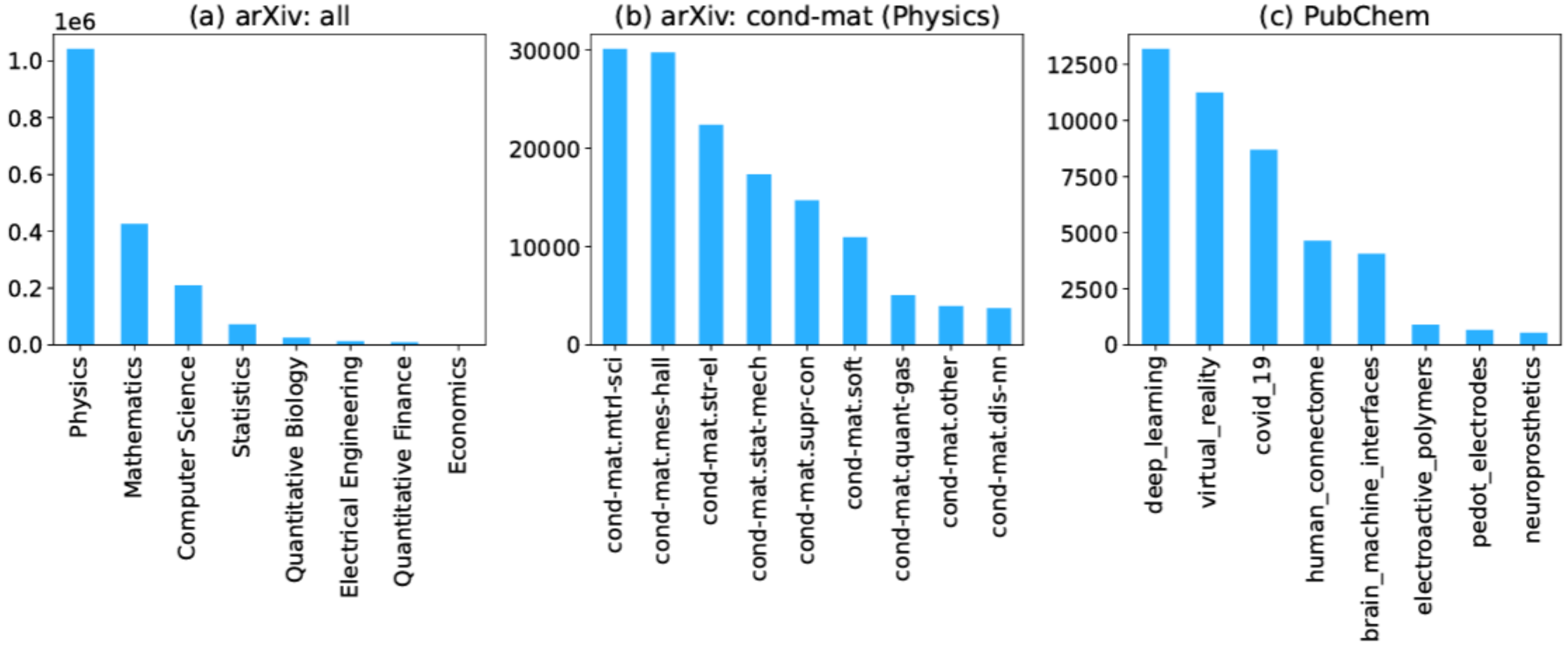
- $TF_{\text{coffee}} = 0.05$
- $IDF_{\text{coffee}} = 2$

The **TF-IDF score** for the term "coffee" is:

$$TF\text{-}IDF_{\text{coffee}} = 0.05 \times 2 = 0.1$$

ChemNLP Datasets

Exploratory data analysis (EDA)



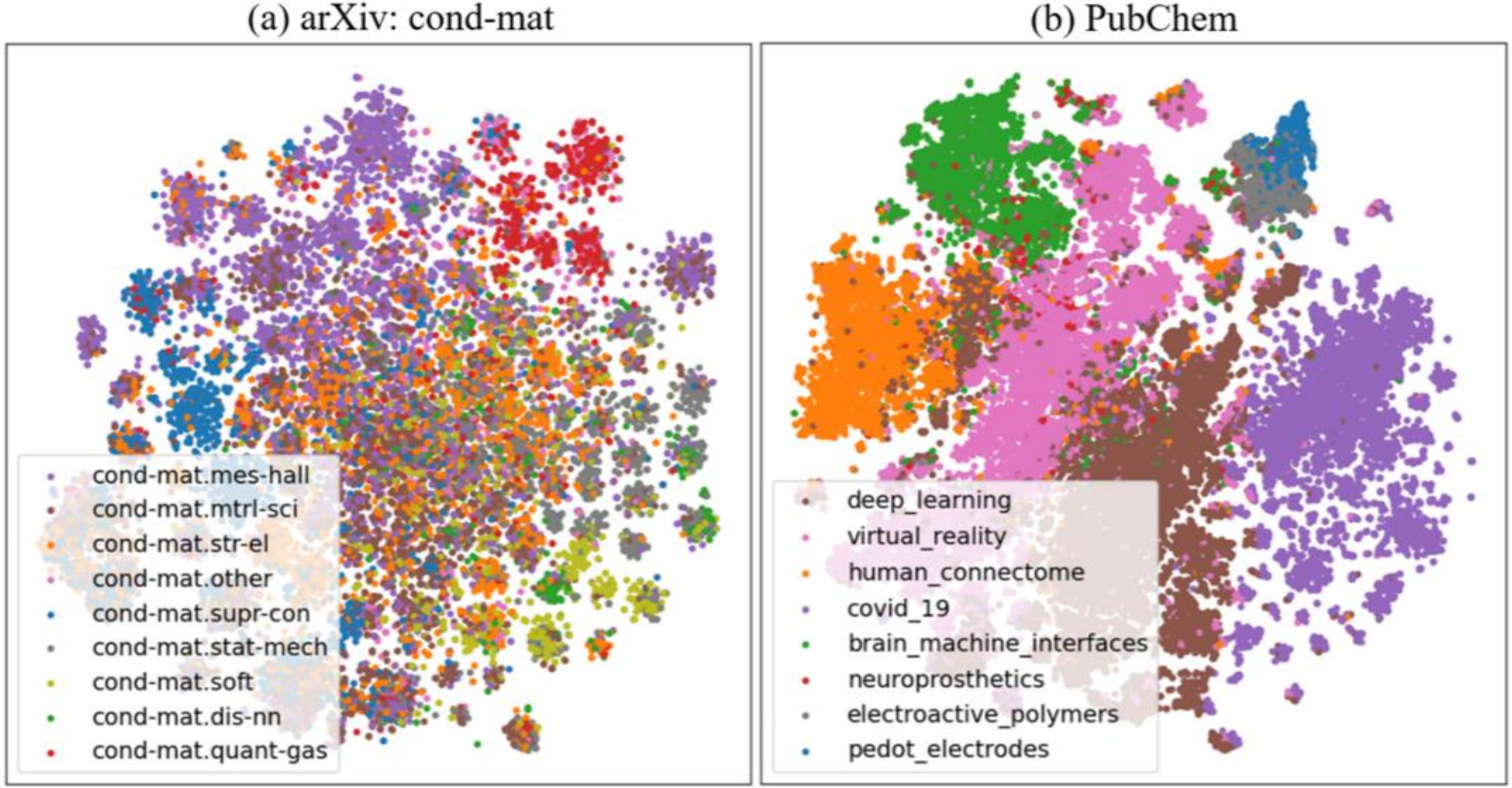


Figure 4: The t-SNE visualisations of the cond.mat articles in the arXiv and PubChem datasets.

Text classification

Accuracy

Table 1: Comparison of models for classifying articles.

	arXiv		
Model	Title only	Abstract only	Title+Abstract
SVM	84.8	90.8	91.3
DistilBert	86.7	89.9	90.0
RF	86.9	88.4	88.6
LR	79.2	85.0	86.0
GNN	76.0	81.0	82.0
	PubChem		
SVM	94.5	94.0	97.6
DistilBert	94.5	97.0	97.5
RF	94.3	94.0	96.7
LR	92.0	93.0	96.7
GNN	85.0	91.0	92.0

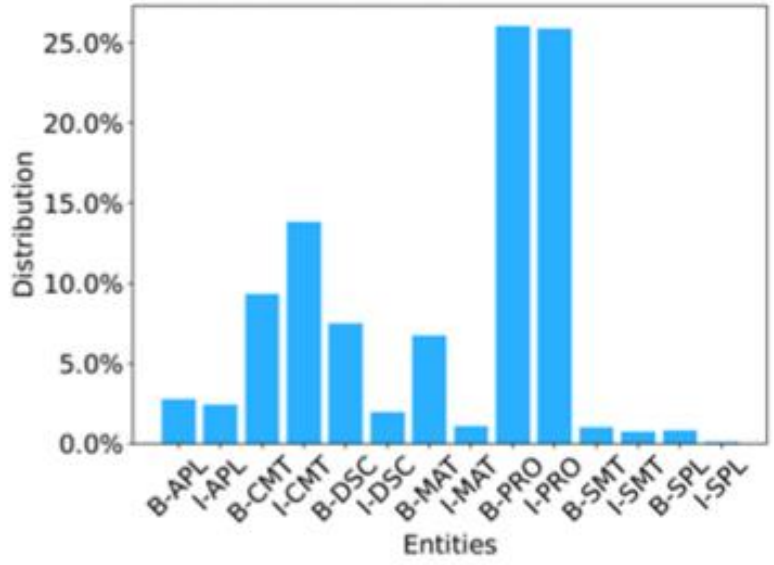
$$Accuracy = \frac{TP + TN}{TP + FN + FP + TN}$$

Named Entity Recognition/Token classification

(a) Example NER application

The electrochemical B-PRO lithium B-MAT -ion extraction/insertion I-PRO properties I-PRO of two spinel B-SPL lithium B-MAT manganese I-MAT oxides I-MAT , stoichiometric B-DSC Li0.99Mn2O4 B-MAT and lithium B-MAT -rich Li1.04Mn1.93O4 B-MAT were studied. Their voltage B-PRO profile I-PRO and cyclic B-CMT voltammetry I-CMT all show two-step reaction for lithium B-MAT -ion extraction/insertion I-PRO at their 4 V plateau. The high-resolution B-CMT in situ X-ray B-CMT diffraction I-CMT (XRD) studies show both materials experience three cubic B-SPL phases, cubic B-SPL I, II, and III, during cycling at 4 V plateaus. Two two-phase coexistence regions were observed. These results show that phase transitions between cubic B-SPL I and II and between cubic B-SPL II and III are first-order transitions. The in situ XRD data also reveal that lithium B-MAT -rich composition does not suppress the phase transitions of spinel B-SPL between their three cubic B-SPL phases, but leads to the increase of variation range of the lattice parameters of the cubic B-SPL phases. This in turn reduces the jumping step of the lattice parameter between adjacent phases and increases the overlap of the adjacent phase. This study shows conclusively that the three-phase process is the intrinsic feature of spinel B-SPL Li1+yMn2O4 during lithium B-MAT -ion extraction/insertion I-PRO on the 4 V plateau.

(b) NER on arXiv cond-mat



The performance of the model is measured in terms of F1 score given by:

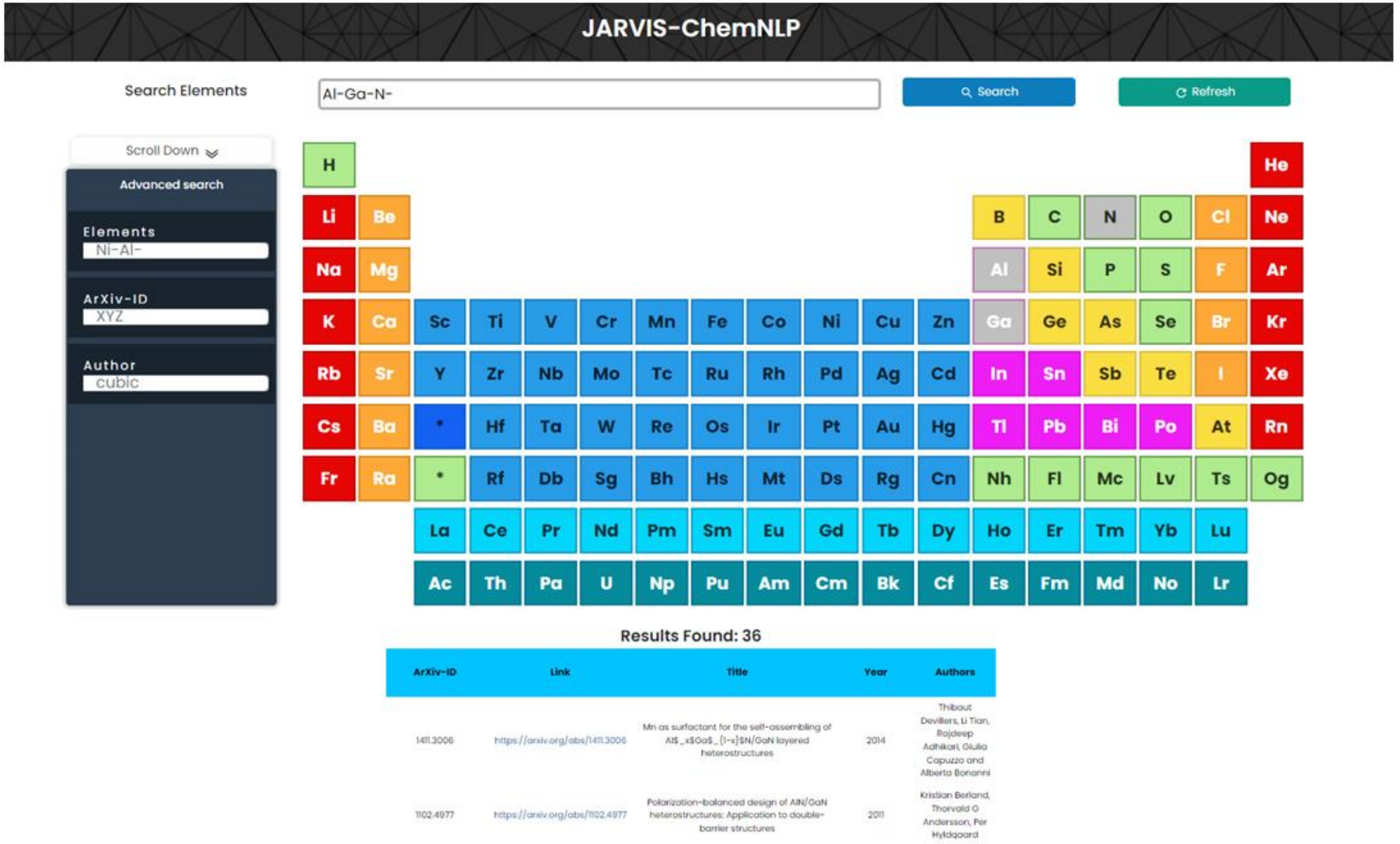
$$F_1 = \frac{2TP}{2TP + FP + TN} \tag{5}$$

where, TP, TN, FN, FP are True Positive, True Negative, False Negative, and False Positive instances respectively. Similar to accuracy, the maximum value of F1 is 100 %.

87 % F1 score

ChemNLP Webpage for Composition Search

https://jarvis.nist.gov/jarvischemnlp/



Introduction to Inverse Materials Design

NIST MATERIAL MEASUREMENT LABORATORY

What is Inverse Materials Design?

- Instead of going from Structure-to-Property, perform **Property-to-Structure** design
- These properties could be: **scalar (e.g. bandgap), spectra (e.g. XRD), image (e.g. STM)**
- Goes beyond **funnel**-like/screening-based materials design

Challenges in Traditional Approaches

- Leads to combinatorial challenge
- Available methods (GA, MC, CE, BO): **limited ability to handle complex** materials spaces
- Lack of well-defined **database** and **benchmarking**
- No unified **physics-based** theoretical model, hence alternative as **AI models**
- Which AI models: **GNN or GPT?**

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Perspective | Published: 29 March 2018

Inverse design in search of materials with target functionalities

Alex Zunger

THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

pubs.acs.org/JPCL Letter

Inverse Design of Next-Generation Superconductors Using Data-Driven Deep Generative Models

Daniel Wines,* Tian Xie, and Kamal Choudhary

THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS
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pubs.acs.org/JPCL Letter

AtomGPT: Atomistic Generative Pretrained Transformer for Forward and Inverse Materials Design

Kamal Choudhary*

Transformer Architecture

Computer Science > Computation and Language

[Submitted on 12 Jun 2017 (v1), last revised 6 Dec 2017 (this version, v5)]

Attention Is All You Need

~140k citations in 7 years

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, Illia Polosukhin

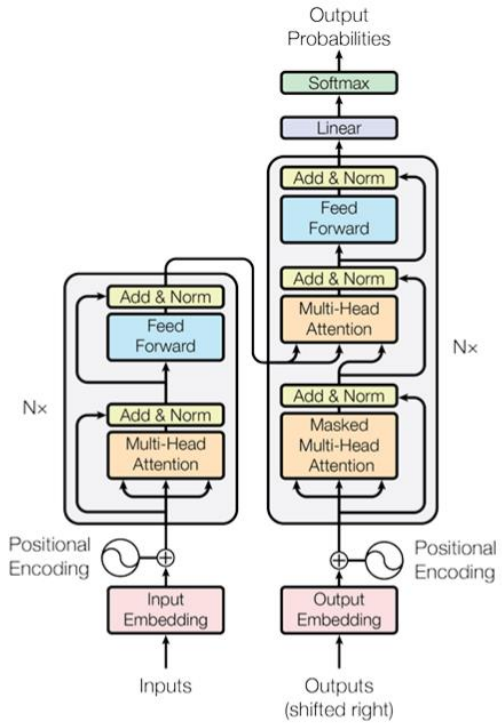
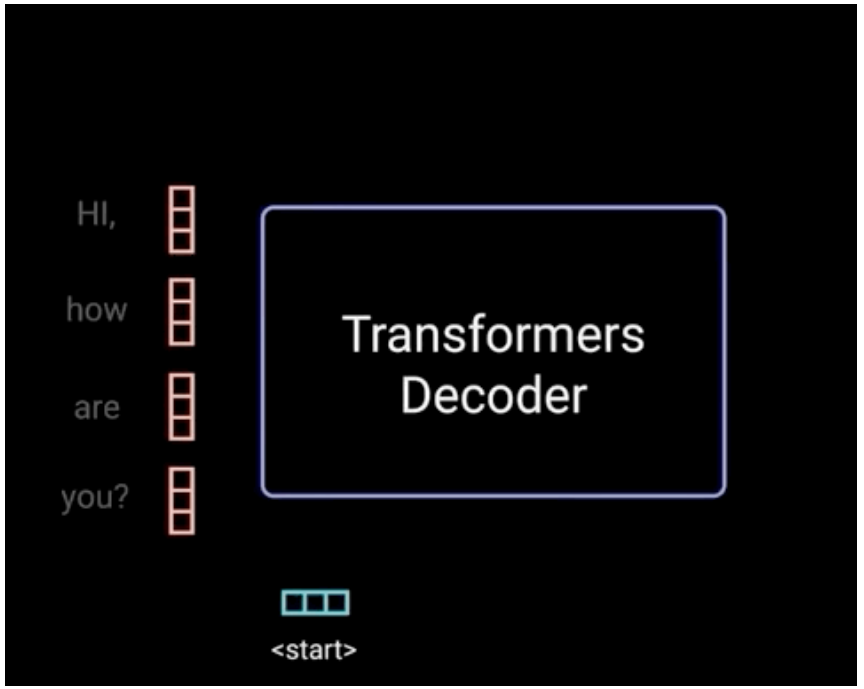


Figure 1: The Transformer - model architecture.



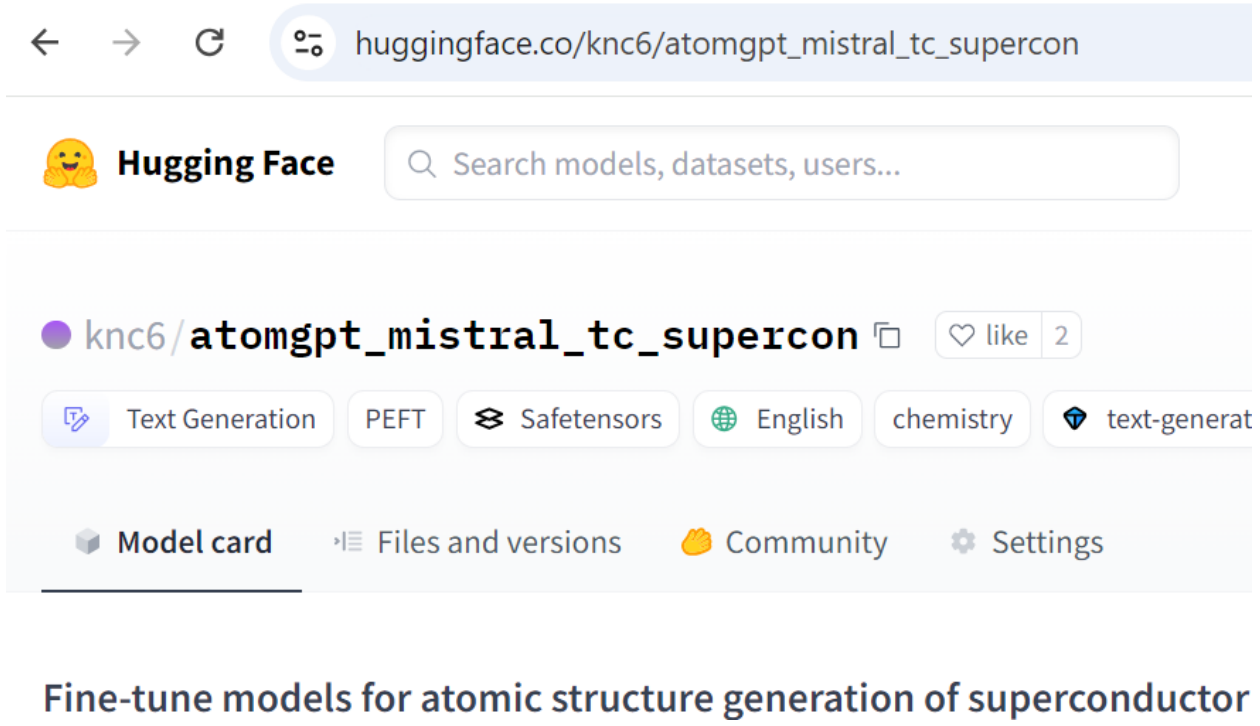
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

Much better than RNN, LSTM etc.

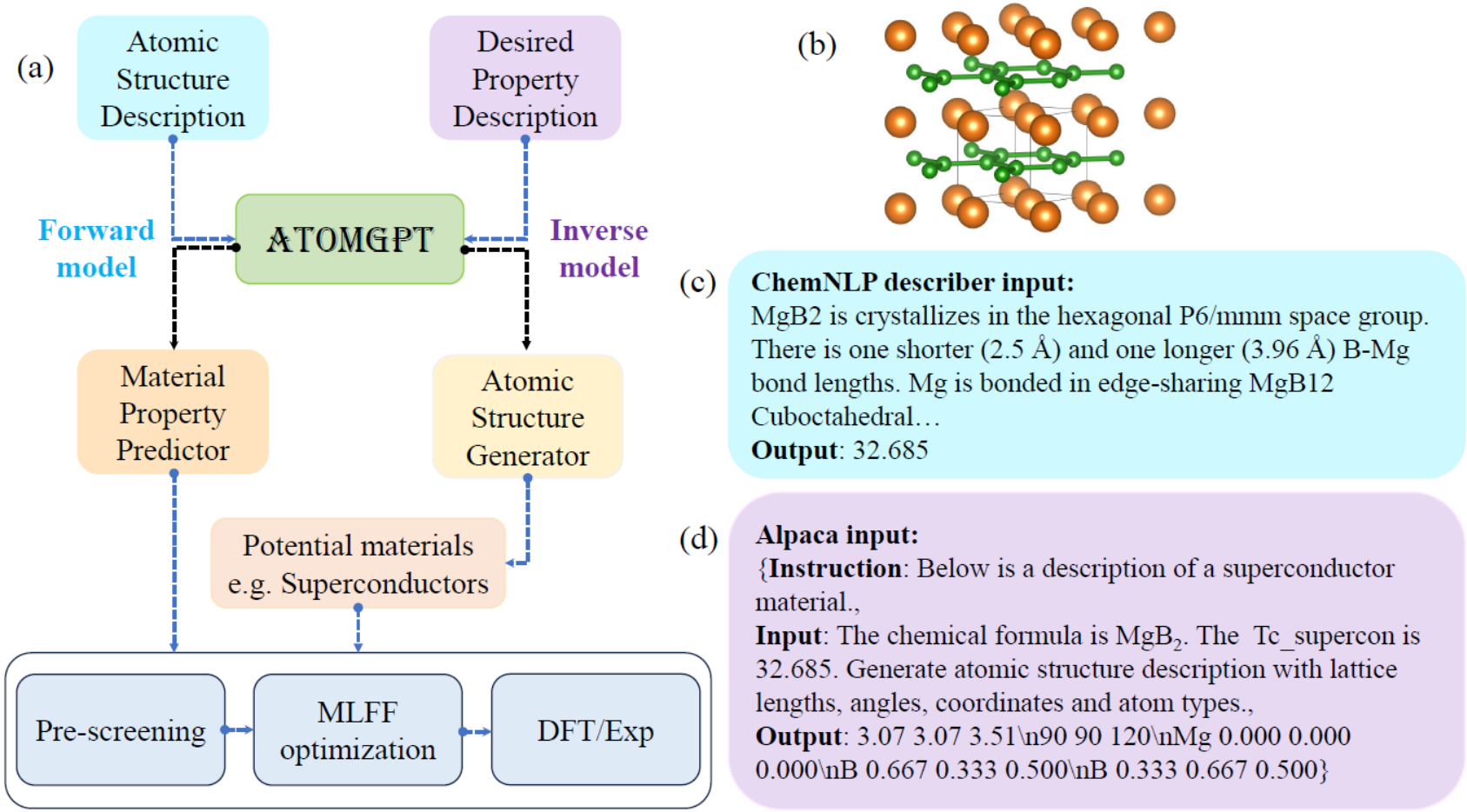
Attention:~ extremely long-term memory

AtomGPT Architecture

- Uses HuggingFace ecosystem https://huggingface.co/
- Uses Mistral AI-7B
- Modified language model head for forward models
- Low-rank adaptation (LoRA) for parameter-efficient fine-tuning (PEFT)
- Rotary position embedding (RoPE)
- Transformer reinforcement learning (TRL)



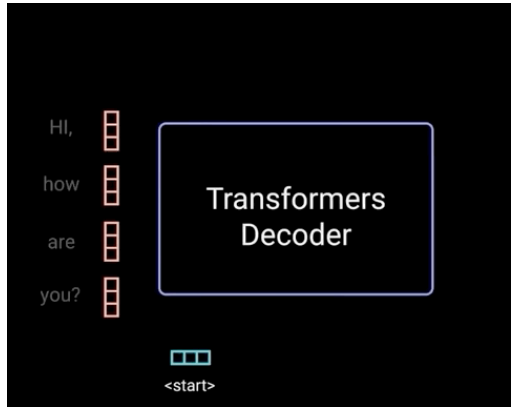
AtomGPT



(b)

(c) **ChemNLP describer input:**
MgB2 is crystallizes in the hexagonal P6/mmm space group. There is one shorter (2.5 Å) and one longer (3.96 Å) B-Mg bond lengths. Mg is bonded in edge-sharing MgB12 Cuboctahedral…
Output: 32.685

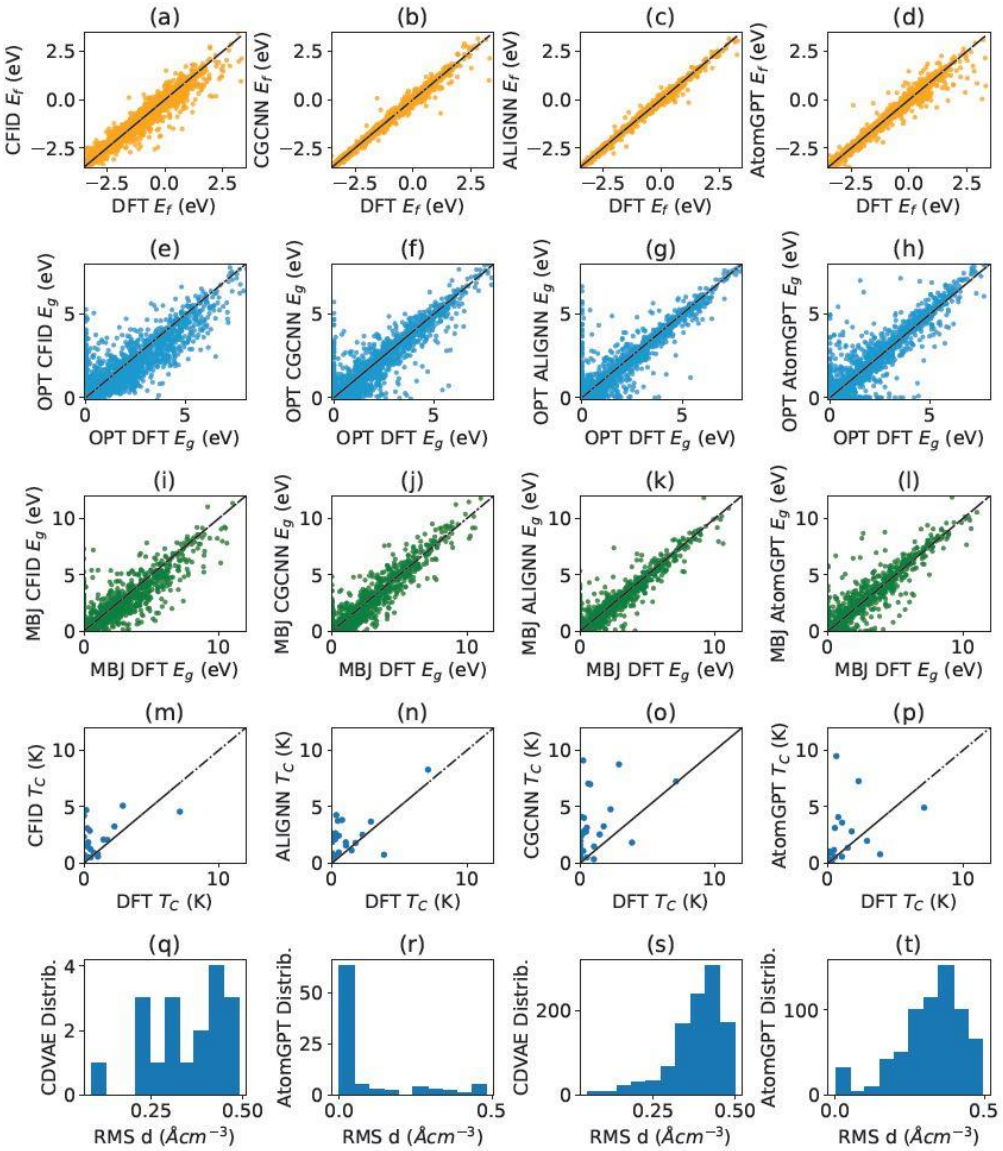
(d) **Alpaca input:**
{**Instruction**: Below is a description of a superconductor material.,
Input: The chemical formula is MgB_2. The Tc_supercon is 32.685. Generate atomic structure description with lattice lengths, angles, coordinates and atom types.,
Output: 3.07 3.07 3.51\n90 90 120\nMg 0.000 0.000 0.000\nB 0.667 0.333 0.500\nB 0.333 0.667 0.500}



$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

AtomGPT: Atomistic Generative Pretrained Transformer for Forward and Inverse Materials Design, J. Phys. Chem. Lett., 2024

AtomGPT



Forward models				
Prop/MAE	CFID	CGCNN	ALIGNN	AtomGPT
E_{form} (eV/atom)	0.142	0.063	**0.033**	0.072
OPT E_g (eV)	0.299	0.199	0.142	**0.139**
MBJ E_g (eV)	0.531	0.407	**0.310**	0.319
T_C (K)	1.99	2.60	2.03	**1.54**

Inverse models		
Database/RMSE	CDVAE	AtomGPT
SuperConDB	0.24	**0.08**
Carbon24	0.36	**0.32**

AtomGPT: Atomistic Generative Pretrained Transformer for Forward and Inverse Materials Design

Kamal Choudhary*

Cite this: *J. Phys. Chem. Lett.* 2024, 15, XXX, 6909−6917

Publication Date: June 27, 2024

https://doi.org/10.1021/acs.jpclett.4c01126

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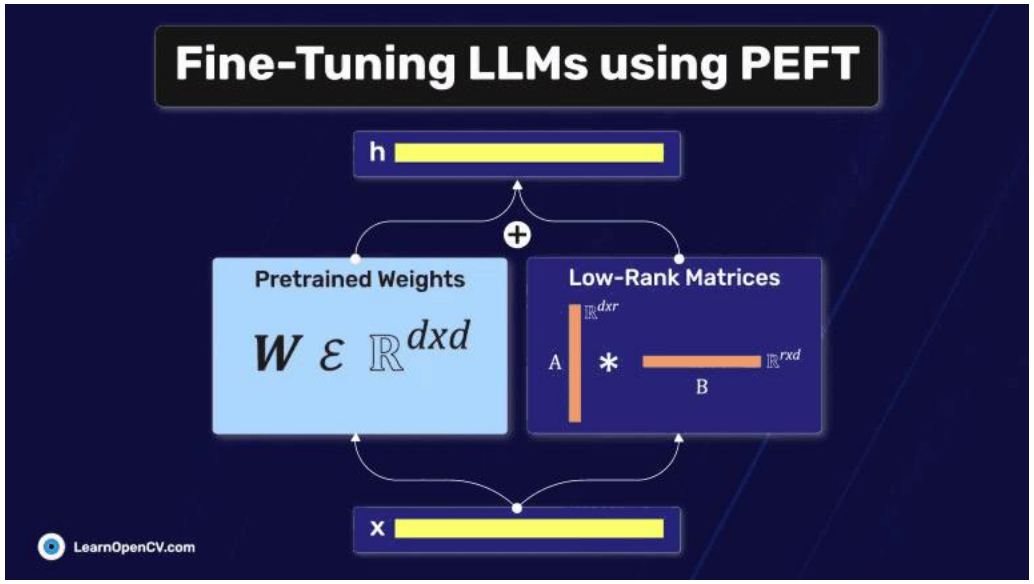
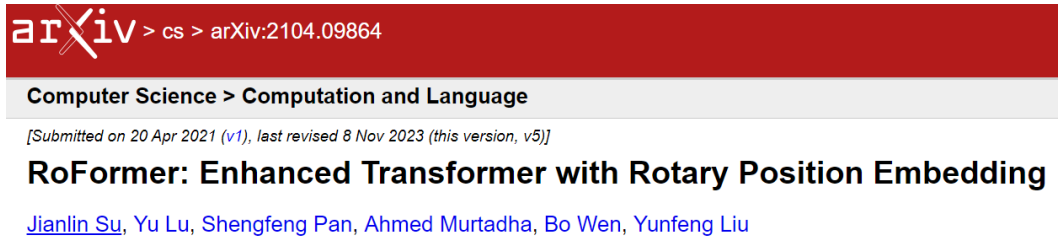
Generated structures relaxed with ALIGNN-FF before DFT-superconductivity workflow

AtomGPT Architecture





Future work:
Integrate AtomGPT with
Retrieval-Augmented Generation (**RAG**)
https://learnopencv.com/fine-tuning-llms-using-peft/

- **Parameter-Efficient Fine-Tuning (PEFT):** adjusting only a subset of parameters while keeping the majority of the model frozen
- **Low-Rank Adaptation (LoRA):** A specific form of PEFT that inserts low-rank matrices into the model's architecture. These matrices capture task-specific knowledge and are fine-tuned while keeping the majority of the model's original parameters fixed.
- **Automatic Mixed Precision (AMP)**: Trains LLMs with mixed-precision data types for faster computations without loss of accuracy.
- **Gradient Accumulation**: Accumulates gradients over multiple batches to reduce memory usage.
- **Transformer Reinforcement Learning** (TRL): transformer architectures based agents for Reinforcement Learning (RL) instead of simple NNs
- **Rotary Position Embedding** (RoPE): encodes the absolute position with a rotation matrix and meanwhile incorporates the explicit relative position dependency in self-attention formulation

Try AtomGPT on Google Colab Today!

NIST MATERIAL MEASUREMENT LABORATORY

Google colab/Jupyter notebook

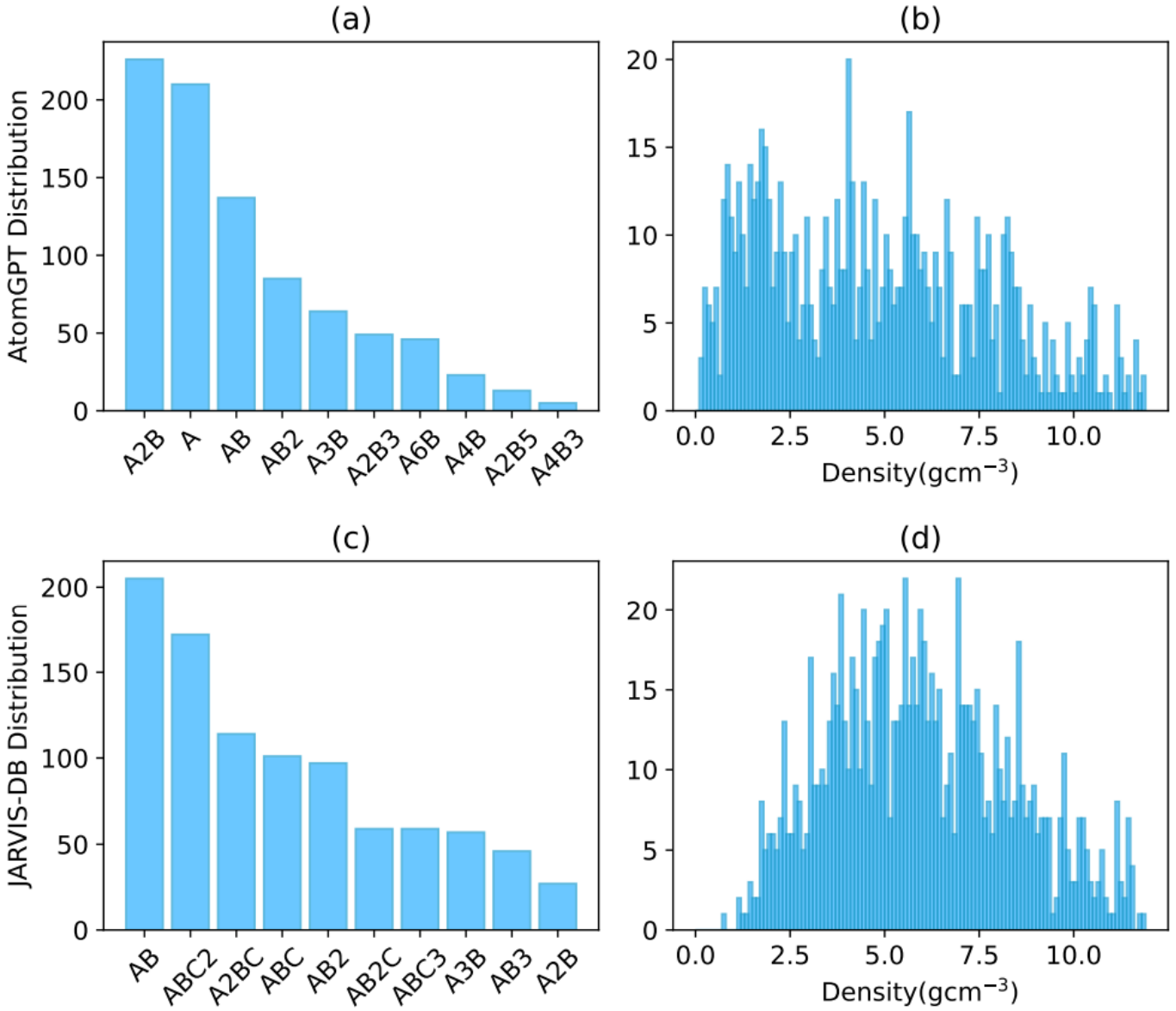
Notebooks	Google Colab	Descriptions
Forward Model training	Open in Colab	Example of forward model training for exfoliation energy.
Inverse Model training	Open in Colab	Example of installing AtomGPT, inverse model training for 5 sample materials, using the trained model for inference, relaxing structures with ALIGNN-FF, generating a database of atomic structures.
HuggingFace model inference	Open in Colab	AtomGPT Structure Generation/Inference example with a model hosted on Huggingface.

For similar other notebook examples, see JARVIS-Tools-Notebook Collection

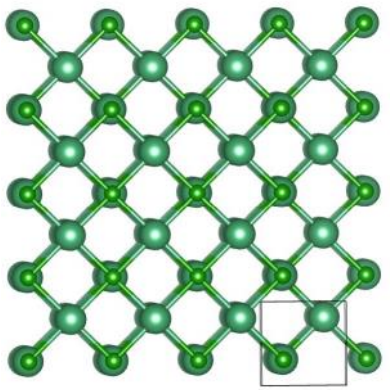
HuggingFace link 🤗 https://github.com/usnistgov/atomgpt

https://huggingface.co/knc6

AtomGPT



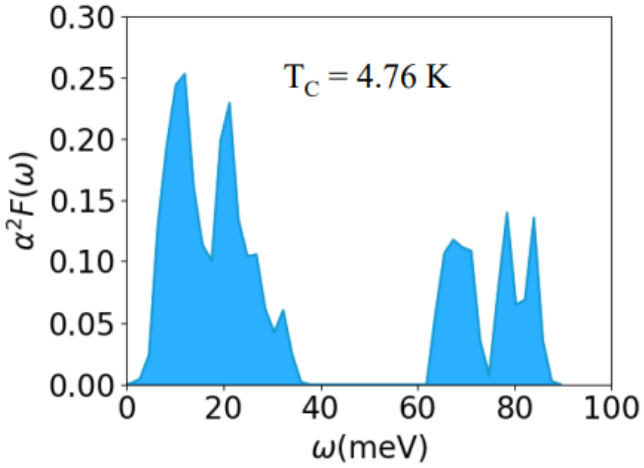
a) Nb_2B structure



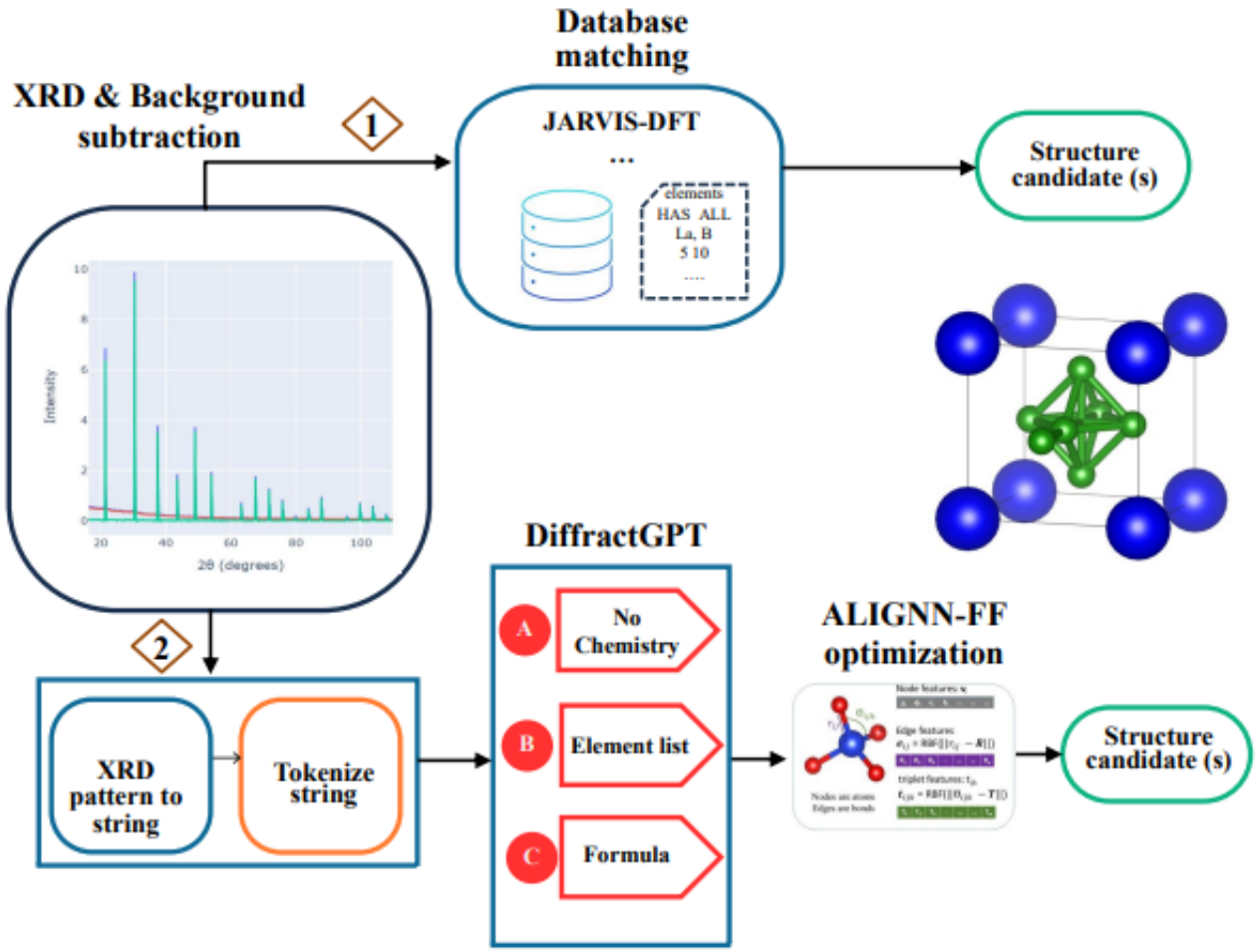
$$T_c = \frac{\omega_{log}}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]$$

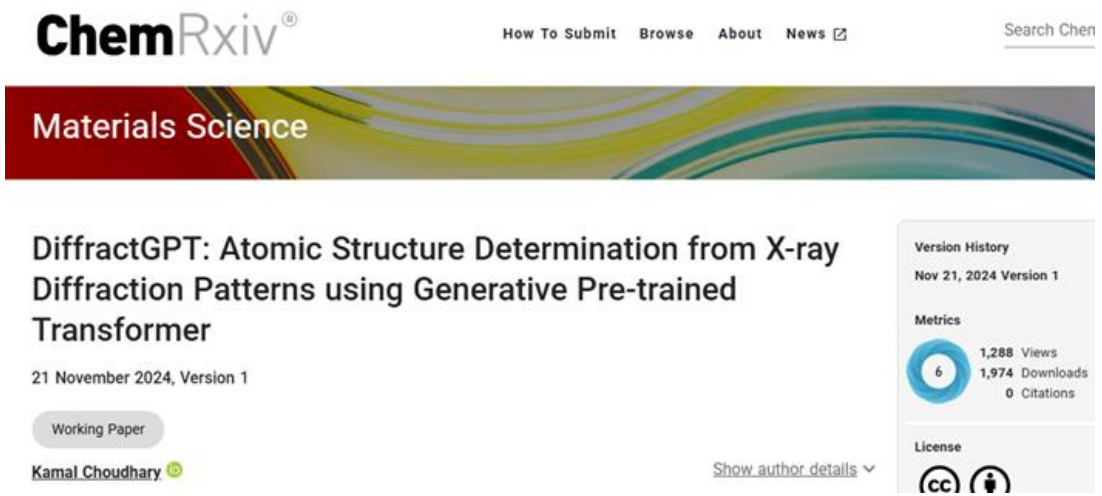
$$\omega_{log} = \exp\left[\frac{\int d\omega \frac{\alpha^2 F(\omega)}{\omega} \ln \omega}{\int d\omega \frac{\alpha^2 F(\omega)}{\omega}}\right]$$

b) Eliashberg function



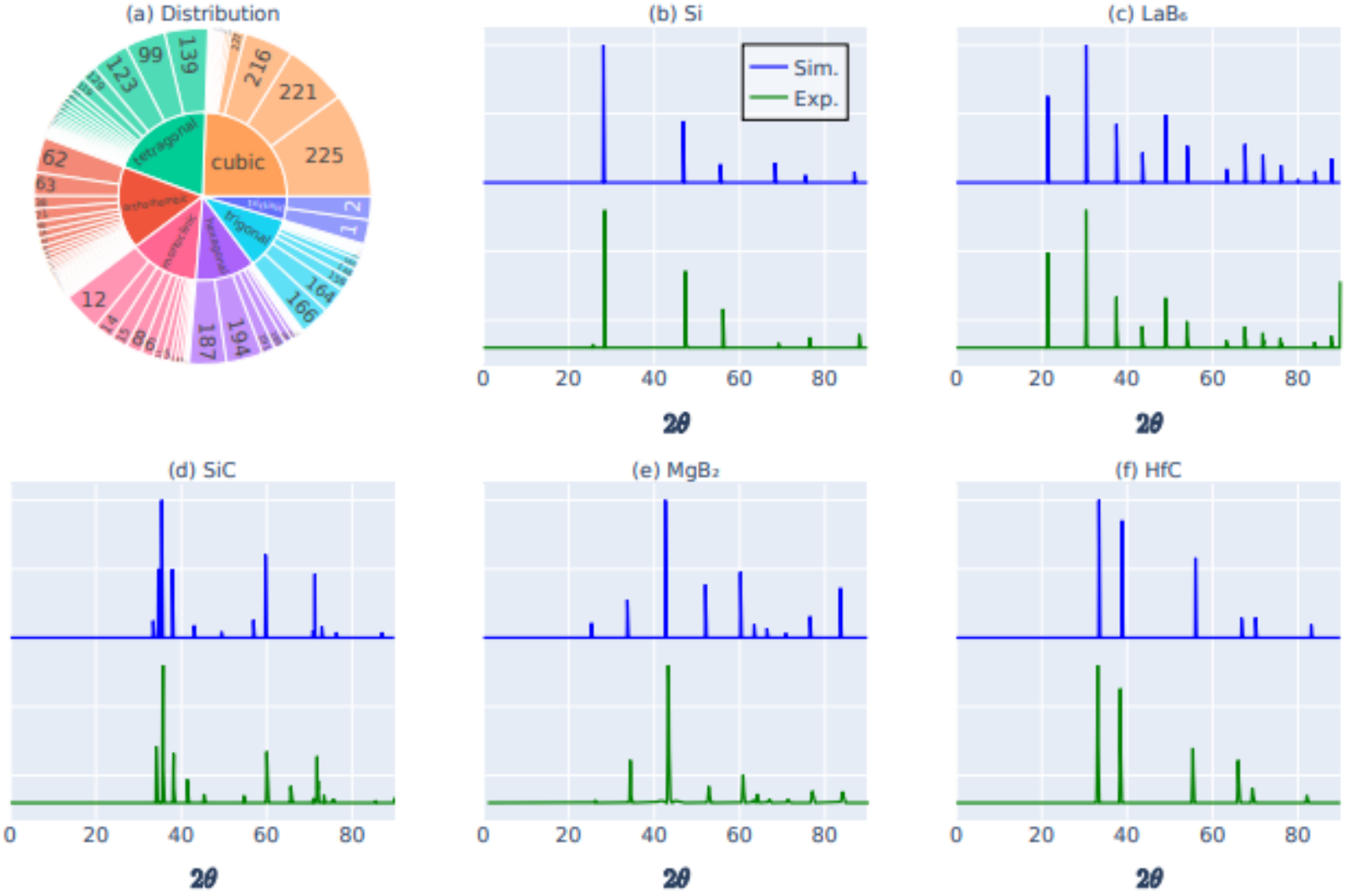
DiffractGPT: AtomGPT for Spectra





Prompt: Here is a spectra of a material "*******", generate lattice matrix, elements and coordinates

DiffractGPT dataset

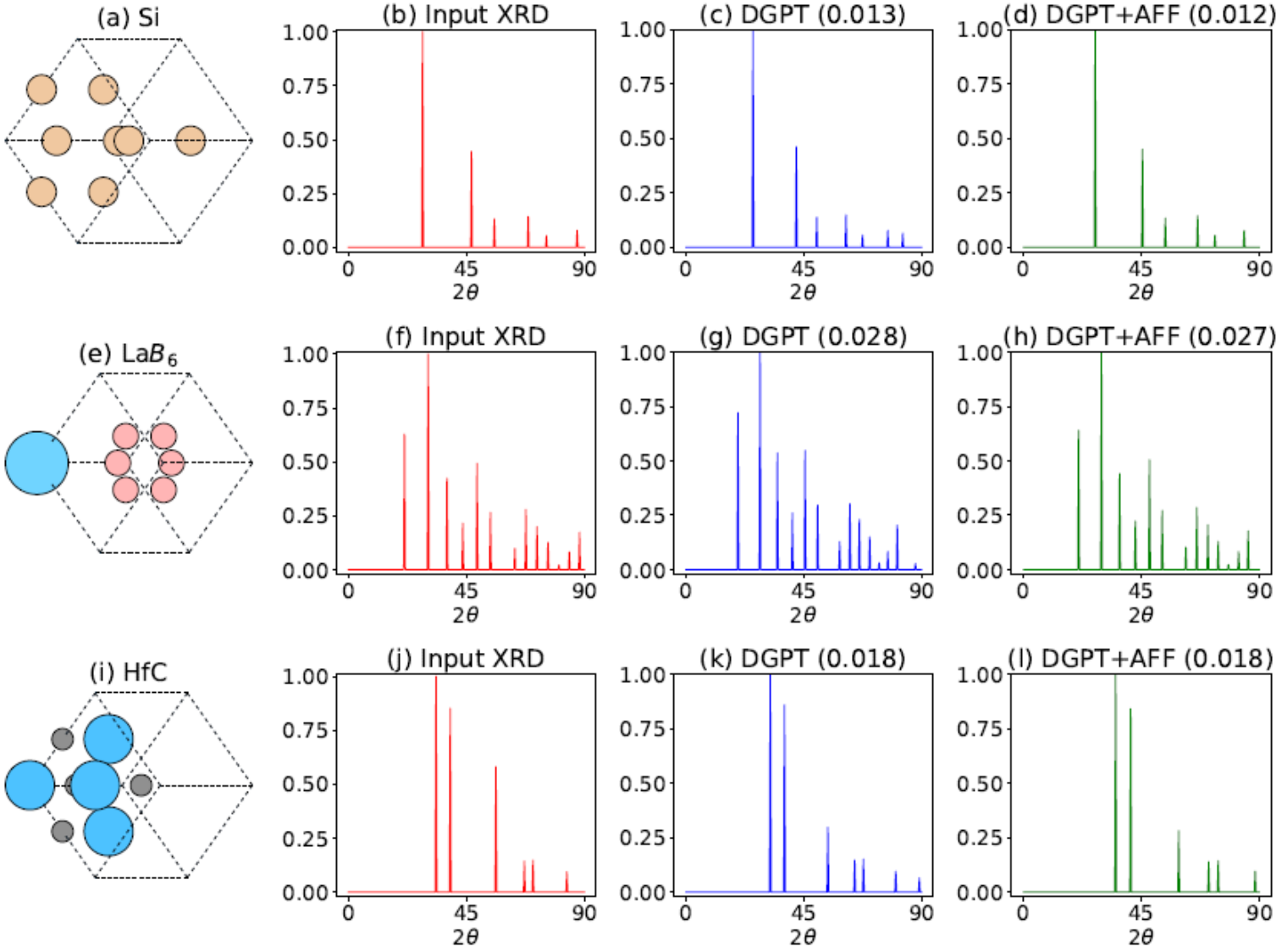


DiffractGPT Performance

Table 1: Performance measurement in terms of mean absolute error (MAE) for predicting lattice constants ($\AA$) using gradient boosting regression (GBR), convolutional neural network (CNN), and varieties of DiffractGPT (DGPT) models. We also compare root mean square distance in predicted vs target structures using DGPT models.

Prop/MAE	GBR	CNN	DGPT-no formula	DGPT-element list	DGPT-formula
a	1.03	0.28	0.25	0.18	**0.17**
b	0.99	0.27	0.26	0.20	**0.18**
c	1.27	0.28	0.38	0.28	**0.27**
RMS-d	-	-	0.23	0.21	**0.07**

DiffractGPT Performance



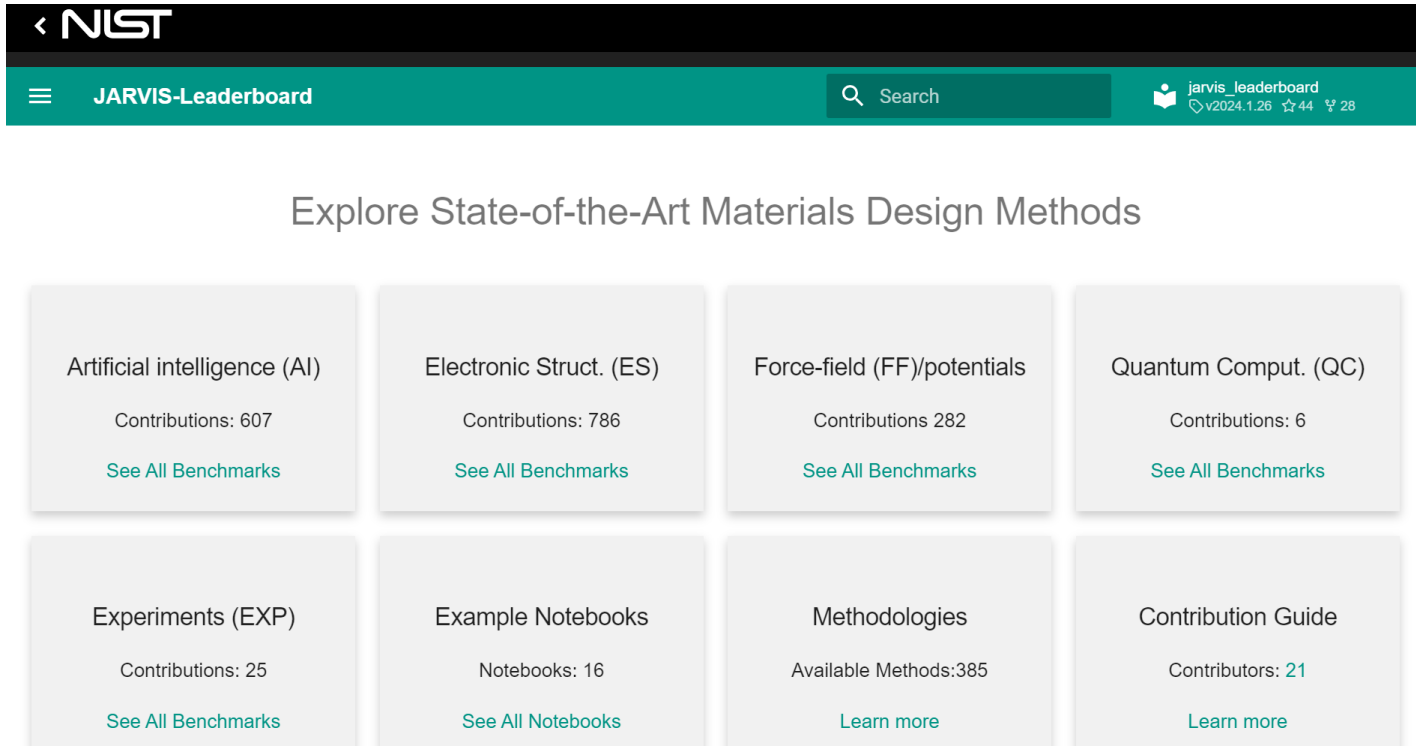
DGPT: DiffractGPT
AFF: ALIGNN-FF

Reproducibility & Benchmarking

Challenges in materials science community:

- Reproducibility
- Transparency
- Validation
- Fidelity
- Data vs. metadata
- What is the ground truth/reference? Synergy of computational and experimental databases

https://pages.nist.gov/jarvis_leaderboard/



1,500 scientists lift the lid on reproducibility

Monya Baker

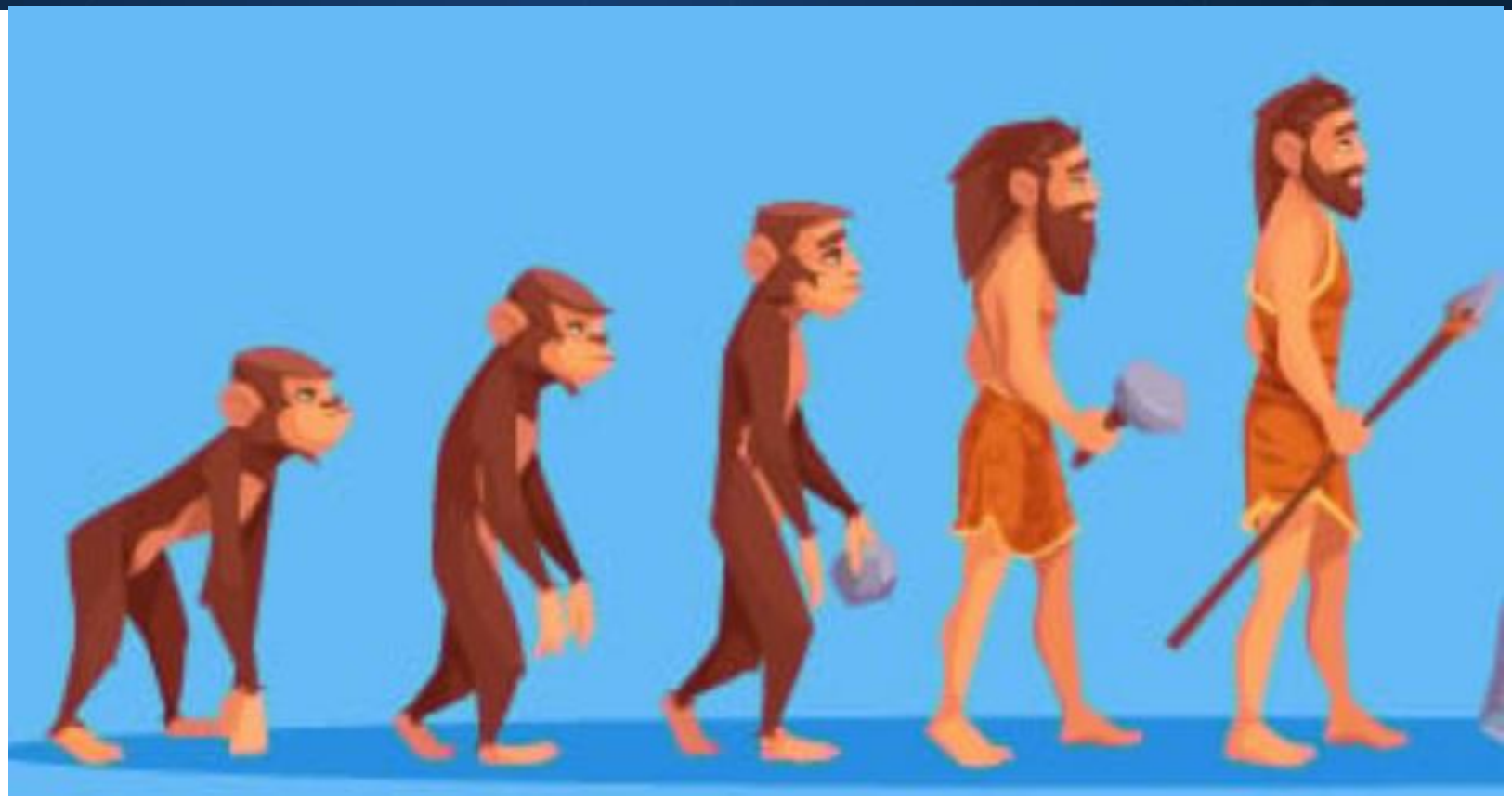
Nature **533**, 452–454 (2016) | Cite this article

171k Accesses | **1952** Citations | **5176** Altmetric | Metrics

Goals

1. Flexibility to add new benchmarks
2. Experimental round-robin studies
3. Multi-modality: benchmarks beyond AI/ML/atomistic property
4. Easy to use/ get started
5. worked out examples (Jupyter/Colab notebooks)

Benchmark evolution in MSE



<1900S	1900's	2000's	2010's	Today
Illustrative example	UCI, MNIST & other repos	Multi-modal data	Big data	Designed benchmarks

https://www.mybiosource.com/learn/complete-guide-to-human-evolution/

Categories of benchmarks

NIST MATERIAL MEASUREMENT LABORATORY

JARVIS-Leaderboard: a large scale benchmark of materials design methods

Kamal Choudhary, Daniel Wines, Kangming Li, Kevin F. Garrity, Vishu Gupta, Aldo H. Romero, Jaron T. Krogel, Kayahan Saritas, Addis Fuhr, Panchapakesan Ganesh, Paul R. C. Kent, Keqiang Yan, Yuchao Lin, Shuiwang Ji, Ben Blaiszik, Patrick Reiser, Pascal Friederich, Ankit Agrawal, Pratyush Tiwary, Eric Beyerle, Peter Minch, Trevor David Rhone, Ichiro Takeuchi, Robert B. Wexler, Arun Mannodi-Kanakkithodi, Elif Ertekin, Avanish Mishra, Nithin Mathew, Mitchell Wood, Andrew Dale Rohskopf, Jason Hattrick-Simpers, Shih-Han Wang, Luke E. K. Achenie, Hongliang Xin, Maureen Williams, Adam J. Biacchi & Francesca Tavazza — Show fewer authors

npj Computational Materials **10**, Article number: 93 (2024) | Cite this article

Category	General name	Method Specification
ES	DFT[64]	VASP[52,53] (PBE[54], LDA[64], OptB88vdW[65], Opt86BvdW[66], TBmBJ[67,68], SCAN[69], r2SCAN[70], HSE06[71])
		QE[72] (PBE[54], PBEsol[73])
		ABINIT[74–76] (PBE[54])
		GPAW[77] (PBE[54], LDA[64], GLLB-sc[78])
	QMC[61]	QMCPACK[79] (DMC[61])
	GW[63]	VASP[52,53] (G_0W_0[63], GW_0[63])
	TB[57]	ThreeBodyTB.jl[59] (Wannier90[80])
AI	Descriptor	CFID[81], MagPie[82], MatMiner[55,83], crystal feature model[84], ElemNet[85–87], IRNet[88–90], BRNet[91,92], SNAP[93]
	Graph-based	ALIGNN[94], CGCNN[95], SchNet[96], AtomVision[97], ChemNLP[98], DimeNet+[99,100], CHGNet[101], M3GNET[102] kgcnn_coGN[103], Potnet[104], Matformer[105]
	Transformers	OPT[106], GPT[15], T5[107]
FF	LJ[108]	LAMMPS[109] (2D-Liquid)
	EAM[110]	LAMMPS[109] (FCC-Al)
	REBO[111]	LAMMPS[109] (Diamond-Si)
	AMBER99sb-ildn[112]	GROMACS[113] (Alanine dipeptide)
	CHARMM36m[114]	GROMACS[113] (α-aminoisobutyric acid)
QC	Algorithms	Qiskit[115] (VQE[116], VQD[117])
		PennyLane[118,119] (VQE[116], VQD[117])
	Circuits	Qiskit[115] (PauliTwo Design[115], SU(2)[115])
EXP	Diffraction	XRD (Bruker D8)
	Manometry	CO_2 adsorption FACT lab[120]
	Vibroscopy	Kevlar FAVIMAT[121]
	Magnetometry	Susceptibility (PPMS)[121]

1) Electronic Structure
2) Artificial Intelligence
3) Force Field
4) Quantum Computation
5) Experiment

Types of Data:

- **Atomic structure** (Molecule, Crystal)
- **Material Property** (Bandgap, bulk modulus)
- **Images** (Microscopy: SEM, TEM, STM)
- **Spectra** (Diffraction: X-ray, Neutron, PL)
- **Text** (Research articles, notebooks, blogs)
- **Eigensolver** (Quantum Computation algorithms)

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Categories of benchmarks

NIST MATERIAL MEASUREMENT LABORATORY

Summary table

Category/Sub-cat.	SinglePropertyPrediction	SinglePropertyClass	MLFF	TextClass	TokenClass	TextSummary	TextGen	AtomGen	ImageClass	Spectra	EigenSolver
AI	418	21	119	18	1	1	3	3	2	1	-
ES	776	-	-	-	-	-	-	-	-	10	-
FF	50	-	-	-	-	-	-	-	-	-	-
QC	-	-	-	-	-	-	-	-	-	-	6
EXP	7	-	-	-	-	-	-	-	-	18	-

- Number of contributors: 20
- Number of methods: 159
- Number of benchmarks: 296
- Number of contributions: 1453
- Number of datapoints: 8731126

Currently:

- ~100 Colab tutorial notebooks
- 296 benchmarks (reference)
- 1705 contributions
- ~9 million datapoints

Contributions & Benchmarks

NIST MATERIAL MEASUREMENT LABORATORY

Contributions		Benchmarks (reference point)
1) Electronic Structure	Error metrics	1) Experiment(s)
2) Artificial Intelligence		2) Test dataset
3) Force Field		3) Electronic Structure
4) Quantum Computation		4) Analytical results
5) Experiment		5) Other Experiments

*Benchmarks must be well-defined with an associated DOI

Contributions & Benchmarks

```
jarvis_leaderboard
├── benchmarks
│   ├── AI
│   │   ├── ImageClass
│   │   │   └── stem_2d_image_bravais_class.json.zip
│   │   ├── MLFF
│   │   │   ├── alignn_ff_db_energy.json.zip
│   │   │   └── ...
│   │   ├── SinglePropertyClass
│   │   │   ├── dft_3d_magmom_oszicar.json.zip
│   │   │   └── ...
│   │   ├── SinglePropertyPrediction
│   │   │   ├── dft_3d_formation_energy_peratom.json.zip
│   │   │   ├── ssub_formula_energy.json.zip
│   │   │   └── ...
│   │   ├── Spectra
│   │   │   └── dft_3d_ph_dos.json.zip
│   │   └── TextClass
│   │       ├── arXiv_categories.json.zip
│   │       └── pubchem_categories.json.zip
│   ├── ES
│   │   ├── SinglePropertyPrediction
│   │   │   ├── dft_3d_Tc_supercon.json.zip
│   │   │   ├── dft_3d_Tc_supercon_JVASP_1151_MgB2.json.zip
│   │   │   ├── dft_3d_bandgap.json.zip
│   │   │   ├── dft_3d_bandgap_JVASP_1002_Si.json.zip
│   │   │   ├── dft_3d_bulk_modulus.json.zip
│   │   │   ├── dft_3d_bulk_modulus_JVASP_1002_Si.json.zip
│   │   │   └── ...
│   │   └── Spectra
│   │       ├── dft_3d_dielectric_function.json.zip
│   │       └── ...
│   ├── EXP
│   │   └── Spectra
│   │       └── dft_3d_XRD_JVASP_19821_MgB2.json.zip
│   ├── FF
│   │   └── SinglePropertyPrediction
│   │       ├── dft_3d_bulk_modulus_JVASP_816_Al.json.zip
│   │       ├── ...
│   │       └── ...
│   └── QC
│       └── EigenSolver
│           └── dft_3d_electron_bands_JVASP_816_Al_WTBH.json.zip
```

```
├── contributions
│   ├── densenet_model
│   │   ├── AI-ImageClass-bravais_class-stem_2d_image-test-acc.csv.zip
│   │   ├── metadata.json
│   │   ├── run.sh
│   │   └── run.py
│   ├── alignn_model
│   │   ├── AI-SinglePropertyClass-magmom_oszicar-dft_3d-test-acc.csv.zip
│   │   ├── AI-SinglePropertyPrediction-formation_energy_peratom-dft_3d-test-mae.csv.zip
│   │   ├── ...
│   │   ├── metadata.json
│   │   ├── run.sh
│   │   ├── run.py
│   │   └── Dockerfile
│   ├── qiskit_vqd_SU2
│   │   ├── QC-EigenSolver-electron_bands_JVASP_816_Al_WTBH-dft_3d-test-multimae.csv.zip
│   │   ├── metadata.json
│   │   ├── run.sh
│   │   └── run.py
│   ├── qmcpack_dmc_pbe
│   │   ├── ES-SinglePropertyPrediction-bulk_modulus_JVASP_890_Ge-dft_3d-test-mae.csv.zip
│   │   ├── ...
│   │   ├── metadata.json
│   │   ├── run.sh
│   │   ├── run.py
│   │   └── metadata.json
│   └── ...
```

Requires:

- Six components in the filename
- metadata.json, run.sh

Benchmarks (json.zip)

```
{"train":
        {"JVASP-57695": 1.55,
         "JVASP-39": 1.55,
         "JVASP-7648": 0.38,
         ...
         },
"test":
        {"JVASP-1408": -0.13,
         "JVASP-1195": 1.55,
         "JVASP-20778": 0.1,
         ...
         },
}
```

Contributions (csv.zip)

```
id,prediction
JVASP-1408,0.54107
JVASP-1195,0.78746
JVASP-20778,0.58677
....
```

Example: AI Formation energy per atom

Model for formation_energy_peratom | Search | jarvis_leaderboard v2024.1.26 ☆44 ⑂28

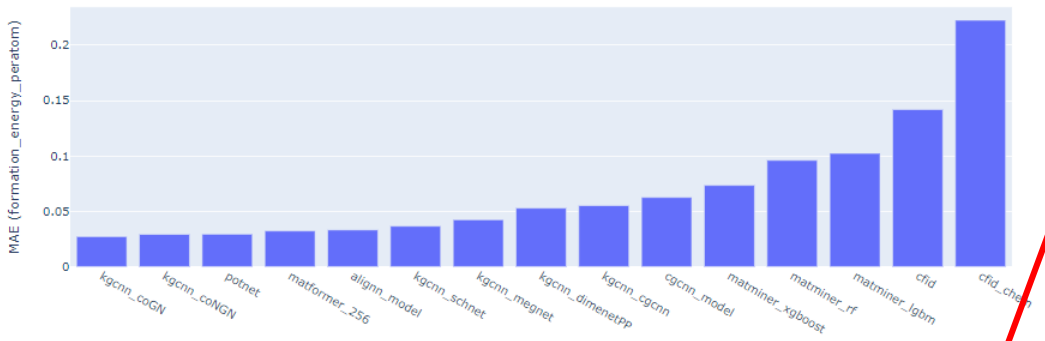
Home | Guide | Notebooks | AI | ES | EXP | FF | QC

AI

- Model for avg_elec_mass
- Model for avg_hole_mass
- Model for bandgap
- Model for bulk_modulus_kv
- Model for dfpt_piezo_max_dielectric
- Model for dfpt_piezo_max_dij
- Model for ehull
- Model for encut
- Model for epsx
- Model for epsy
- Model for epsz
- Model for exfoliation_energy
- Model for formation_energy_peratom
- Model for kpoint_length_unit
- Model for magmom_oszicar
- Model for max_efg
- Model for mbj_bandgap
- Model for mepsx
- Model for mepsy
- Model for mepsz
- Model for n-Seebeck
- Model for n-powerfact
- Model for optb88vdw_bandgap
- Model for optb88vdw_total_energy
- Model for heat capacity
- Model for shear_modulus_gv
- Model for slme
- Model for spillage
- Model for halide perovskite HSE decomposition energy

- Description: This is a benchmark to evaluate how accurately an AI model can predict the formation energy per atom using the JARVIS-DFT (dft_3d) dataset. The dataset contains different types of chemical formula and atomic structures. Here we use mean absolute error (MAE) to compare models with respect to DFT accuracy.

AI-SinglePropertyPrediction-formation_energy_peratom-dft_3d-test-mae



Reference(s): https://www.nature.com/articles/s41524-023-01012-9;https://hackingmaterials.lbl.gov/matminer, https://hackingmaterials.lbl.gov/matminer/, https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.120.145301, https://www.nature.com/articles/s41524-021-00650-1, https://github.com/divelab/AIRS/tree/main/OpenMat/Matformer, https://doi.org/10.1103/PhysRevMaterials.2.083801, https://doi.org/10.48550/arXiv.2305.11842, https://www.nature.com/articles/s41524-020-00440-1, https://github.com/aimat-lab/gcnn_keras, https://github.com/divelab/AIRS/tree/main/OpenMat/PotNet

Model benchmarks

Model name	Dataset	MAE	Team name	Dataset size	Date submitted	Notes
kgcnn_coGN	dft_3d	0.0271	kgcnn	55713	05-06-2023	CSV, JSON, run.sh, Info
kgcnn_coNGN	dft_3d	0.0291	kgcnn	55713	05-06-2023	CSV, JSON, run.sh, Info
potnet	dft_3d	0.0293	DIVE@TAMU	55713	06-02-2023	CSV, JSON, run.sh, Info

	A	B	C	D	E	F	G	H	I	J
1	id	prediction								
2	JVASP-386	-0.06485								
3	JVASP-697	-0.53265								
4	JVASP-120	-0.07311								
5	JVASP-833	-1.86553								
6	JVASP-229	-4.28398								
7	JVASP-120	-0.9024								
8	JVASP-120	-1.56657								
9	JVASP-181	-0.41461								

dft_3d_formation_energy_peratom.json - Notepad

File Edit Format View Help

{"train": {"JVASP-21450": -0.50496, "JVASP-66320": 0.417,
, "JVASP-42000": -0.38536, "JVASP-115193": -0.74961, "JVASI
02245, "JVASP-18480": -2.9647, "JVASP-107218": -0.66397, "
, "JVASP-123687": -0.31591, "JVASP-82029": -0.31863, "JVASI
SP-52188": -2.30026, "JVASP-75687": 0.4939, "JVASP-41702":


```
#!/bin/bash
pip install alignn
python run.py
```


```
{
    "model_name": "ALIGNN",
    "project_url": "https://www.nature.com/articles/s41524-021-00650-1",
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    "author_email": "knc6@nist.gov",
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    "team_name": "ALIGNN",
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Day 4 Hands on

AI 11 JARVIS_Leaderboard_contribution_ALIGNN

AI 12 JARVIS_Leaderboard_MLFF/ALIGNN-FF for Silicon

AI 37 ALIGNN-FF Unified force-field structure relaxation/Phonons/Interface

AI 38 ALIGNN Melt-Quench MD

AI 26 AtomVision Leaderboard Example

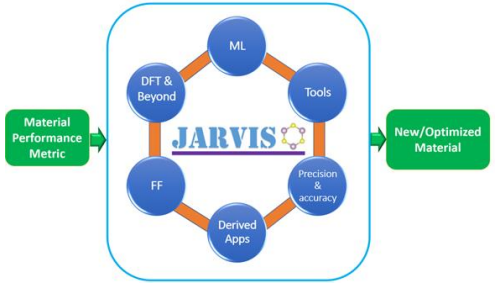
AI 28 ChemNLP Example

AI 31 AtomGPT forward model

AI 33 AtomGPT inverse model

Conclusion and Contact Information

- **NIST-JARVIS Database**: A repository of materials data for research and modeling.
- **Data-modalities:** scalar, spectra, image, text
- **ALIGNN**: Graph neural networks for materials
- **AtomGPT**: Large Language model for inverse materials design and property prediction
- **DiffractGPT**: A generative AI model for XRD to structure
- **JARVIS-Leaderboard**: A benchmarking tool for comparing methods/models on materials design tasks.



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