Introduction to Data Science in Materials Science

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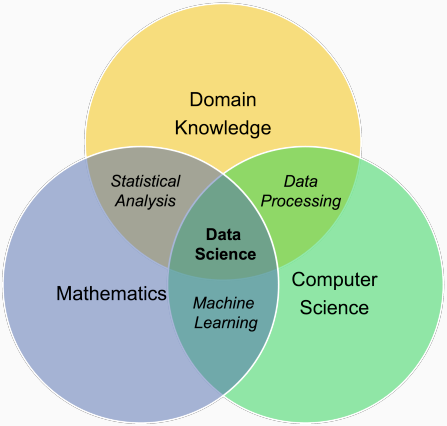
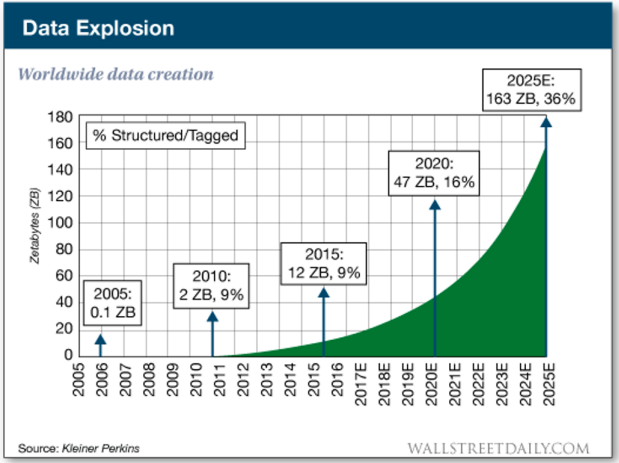
What is Data Science?

Data science is a multi-disciplinary field that uses scientific methods, processes, algorithms and systems to extract knowledge and insights from structured and unstructured data.

What is Data Science?



The Data Age


Data Explosion
Worldwide data creation
2025E:
163 ZB, 36%
% Structured/Tagged
2020:
47 ZB, 16%
2015:
12 ZB, 9%
2010:
2 ZB, 9%
2005:
0.1 ZB
Zetabytes (ZB)
180
160
140
120
100
80
60
40
20
0
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017E
2018E
2019E
2020E
2021E
2022E
2023E
2024E
2025E
Source: Kleiner Perkins
WALLSTREETDAILY.COM

Growth in Materials Data (as of Jan 1 2020)

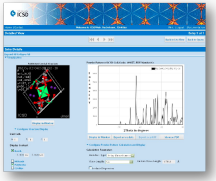


Figure 1: ICSD: ∼200,000 crystals

Figure 2: COD: ∼400,000 crystals

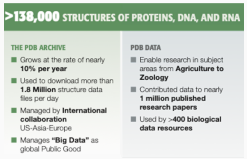


Figure 3: Protein data bank

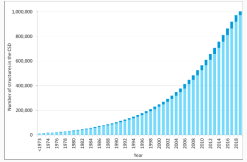


Figure 4: Cambridge structural database (small-molecule organic crystal structures)

But Quantity and Quality Lags Many Other Fields

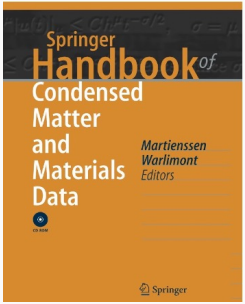


Figure 5: One of the most comprehensive handbooks on materials data: Density, thermal and electrical conductivity, melting and boiling points, etc., but O(100) binaries and limited ternaries...

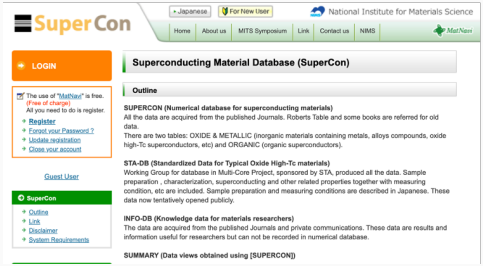
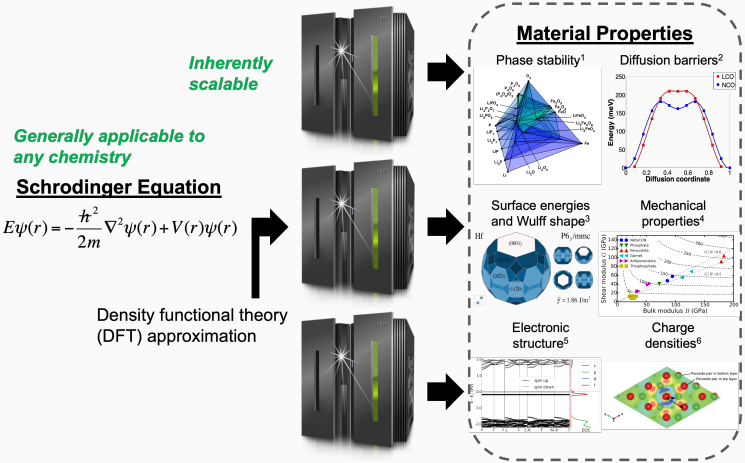
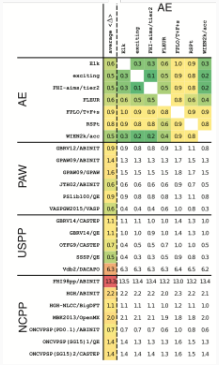


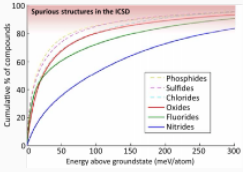
Figure 6: ∼1000+ superconductors (many minor composition modifications). Ref: https://supercon.nims.go.jp/

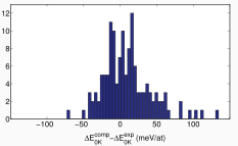
First Principles Materials Computations

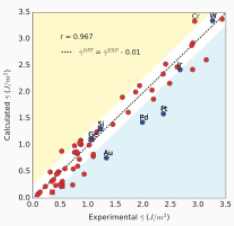


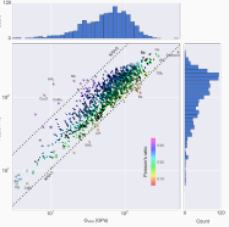
Electronic structure calculations are today reliable and reasonably accurate...









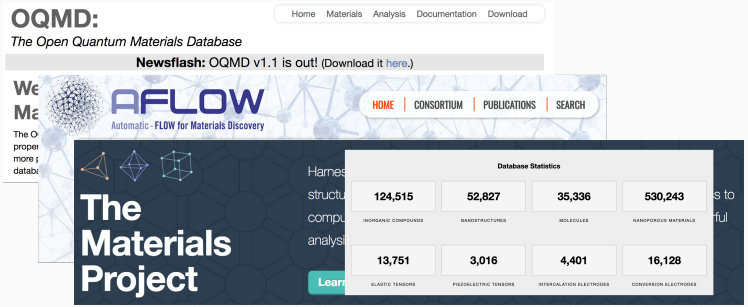


- (left) Modern electronic structure codes give relatively consistent equations of state.
- (right, clockwise from top left) Good predictions can be obtained for phase stability,[1] formation energies, surface energies,[2] and elastic constants[3].

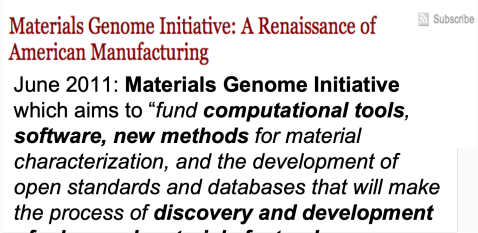
Software frameworks for high-throughput computational materials science

- Materials Project (https://materialsproject.org)[4]
  - Python Materials Genomics or pymatgen (https://pymatgen.org)[5]
  - Custodian (https://materialsproject.github.io/custodian/)
  - FireWorks [6]
- Atomic Simulation Environment (https://wiki.fysik.dtu.dk/ase)
- AFLOW (http://aflowlib.org)[7]
- AiiDa (http://www.aiida.net)

Computation + Automation → Large databases

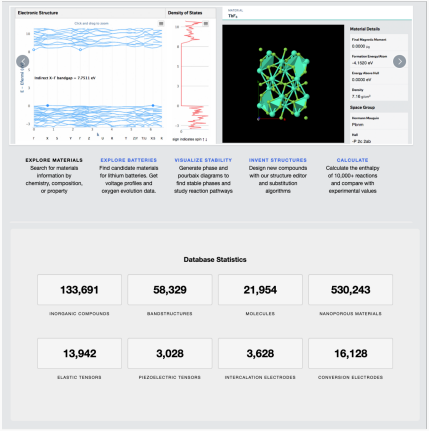


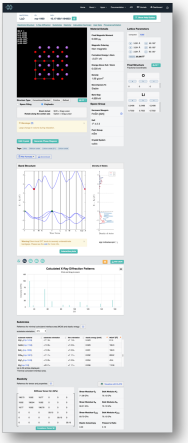
Google for Materials



The Materials Project is an open science project to make the computed properties of all known inorganic materials publicly available to all researchers to accelerate materials innovation.

Google for Materials





Materials Application Programming Interface (API)[8]

- An open platform for accessing Materials Project data based on REpresentational State Transfer (REST) principles.
- *Flexible and scalable* to cater to large number of users, with different access privileges.
- Simple to use and code agnostic.
- Requires an API key, available at: `https://www.materialsproject.org/dashboard`
- Documentation: `https://api.materialsproject.org/docs`

RESTful API

A REST API maps a URL to a resource.

Example

GET https://api.dropbox.com/1/account/info

Returns information about a user's account.

Methods: GET, POST, PUT, DELETE, etc.

Response: Usually JSON or XML or both

Materials API Example

URL

https://api.materialsproject.org/summary/?formula=Fe2O3&_fields=formation_energy_per_atom

Example response:


```
{
    "data":[
        {"_id":"61a2dcaa2c86325a0218b5ef","formation_energy_per_atom":-1.6299189062500006},
        {"_id":"61a2dcb52c86325a021af9bd","formation_energy_per_atom":-1.4175868379999996},
        ...
    ],
    "meta":{
        "api_version":"0.48.0",
        "time_stamp":"2022-09-19T13:17:11.321756",
        "total_doc":26,
        "max_limit":1000,
        "default_fields":["material_id"]
    }
}
```


- Intuitive response format.
- Machine-readable (JSON parsers available for most programming languages).
- Metadata provides provenance for tracking.

Types of Materials Data

Qualitative data

- Nominal measurement.
- E.g., Metal/Insulator, Stable/Unstable.
- No rank or order.

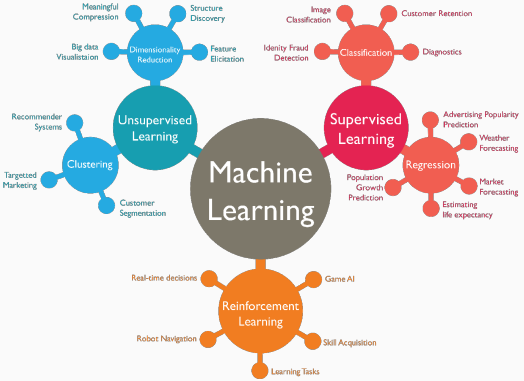
Ranked data

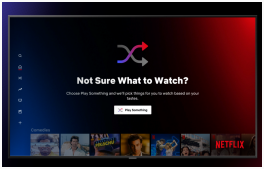
- Ordinal measurement (ordered).
- E.g., Insulator/ semiconductor/ conductor.
- Does not indicate distance between ranks.

Quantitative Data

- Interval/ratio measurement (equal intervals and true 0).
- E.g., melting point, elastic constant, electrical/ionic conductivity.
- Considerable information and permits meaningful arithmetic operations.

What is Machine Learning?





Nobel Prizes in Chemistry and Physics 2024

The Nobel Prize in Chemistry 2024

David Baker

"for computational protein design"

David Baker. Ill. Niklas Elmehed © Nobel Prize Outreach

Demis Hassabis

"for protein structure prediction"

Demis Hassabis. Ill. Niklas Elmehed © Nobel Prize Outreach

John Jumper

"for protein structure prediction"

John Jumper. Ill. Niklas Elmehed © Nobel Prize Outreach

The Nobel Prize in Physics 2024

John Hopfield

"for foundational discoveries and inventions that enable machine learning with artificial neural networks"

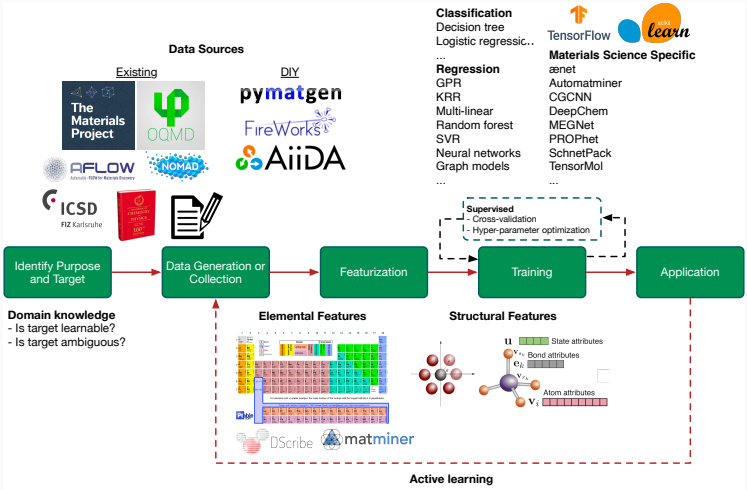
John Hopfield. Ill. Niklas Elmehed © Nobel Prize Outreach

Geoffrey Hinton

"for foundational discoveries and inventions that enable machine learning with artificial neural networks"

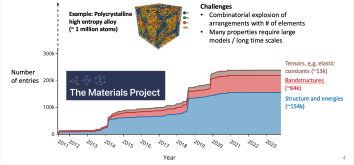
Geoffrey Hinton. Ill. Niklas Elmehed © Nobel Prize Outreach

Materials ML Workflow

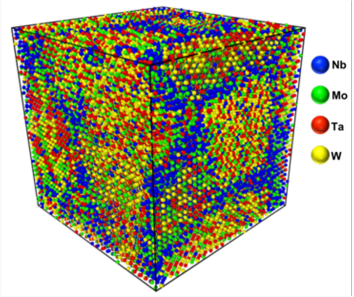


Where is ML valuable in Materials Science?

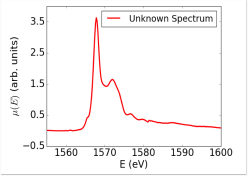
Too many to compute

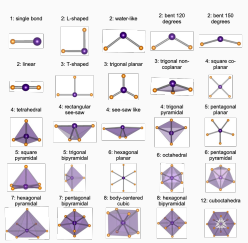


Too big to compute

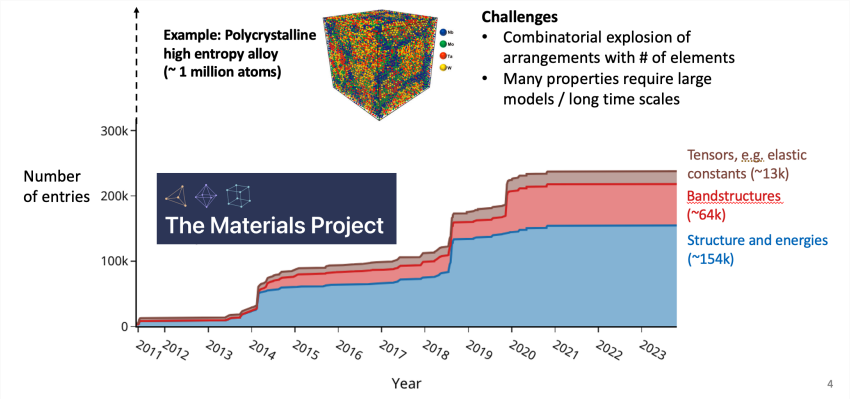


Too complex to understand.





Data History of the Materials Project



Surrogate models for “instant” property predictions

$$\text{Property} = f(\text{Composition}, \text{Structure})$$

- The material property, e.g., energetic (formation, energy above hull, reaction, etc.), electronic (band gaps, DOS), mechanical, functional (e.g., ionic conductivity) is called the **“target”**.
- Composition and Structure are called the **“descriptors”** or **“features”**.
- Examples of compositonal features: stoichiometric attributes, e.g., # and ratio of elements; elemental properties, e.g., mean, range, min, max of atomic number, electronegativity, row, group, radii, # of valence electrons, etc.
- Examples of structural features: crystal/molecular symmetry, lattice parameters, atomic coordinates, connectivity / bonding between atoms.

Compositional features

- **Average atomic mass**: Composition-weighted average of the atomic masses of the elements in the compound. *Value for FeO: 0.5 x 55.845 + 0.5 x 15.999 = 35.92.*
- **Average column on periodic table**: Composition-weighted average of the columns of the elements in the compound. *Value for FeO: 0.5 x 8 + 0.5 x 16 = 12.0.*
- **Average row on the periodic table**: Composition-weighted average of the rows of the elements in the compound. *Value for FeO: 0.5 x 4 + 0.5 x 2 = 3.0.*
- **Maximum difference in atomic number**: Largest atomic number in the composition less the smallest. *Value for FeO: 26 – 8 = 18.*
- **Average atomic number**: Composition-weighted average of the atomic numbers of the elements in the compound. *Value for FeO: 0.5 x 26 + 0.5 x 8 = 17.0.*
- **Maximum difference in atomic radii**: Largest atomic radius in the composition less the smallest (in pm). *Value for FeO: 140 – 60 = 80.*
- **Average atomic radius**: Composition-weighted average of the atomic radii of the elements in the compound. *Value for FeO: 0.5 x 140 + 0.5 x 60 = 100.0.*
- **Maximum difference in electronegativity**: Largest electronegativity in the composition less the smallest. *Value for FeO: 3.44 – 1.83 = 1.61.*
- **Average electronegativity**: Composition-weighted average of the electronegativities of the elements in the compound. *Value for FeO: 0.5 x 3.44 + 0.5 x 1.83 = 2.635.*
- **Average number of s valence electrons**: Composition-weighted average of the number of s valence electrons associated with the elements in the compound. *Value for FeO: 0.5 x 4 + 0.5 x 2 = 3.0.*
- **Average number of p valence electrons**: Analogous to above, but for *p* electrons. *Value for FeO: 0.5 x 0 + 0.5 x 4 = 2.0.*
- **Average number of d valence electrons**: Analogous to above, but for *d* electrons. *Value for FeO: 0.5 x 6 + 0.5 x 0 = 3.0.*
- **Average number of f valence electrons**: Analogous to above, but for *f* electrons. *Value for FeO: 0.5 x 0 + 0.5 x 0 = 0.0.*
- **s fraction of valence electrons**: Composition-weighted fraction of all valence electrons in the compound that represent s states. *Value for FeO: 3.0 / (3.0 + 2.0 + 3.0 + 0.0) = 0.375.*
- **p fraction of valence electrons**: Analogous to above, but for *p* electrons. *Value for FeO: 2.0 / (3.0 + 2.0 + 3.0 + 0.0) = 0.25.*
- **d fraction of valence electrons**: Analogous to above, but for *d* electrons. *Value for FeO: 3.0 / (3.0 + 2.0 + 3.0 + 0.0) = 0.375.*
- **f fraction of valence electrons**: Analogous to above, but for *f* electrons. *Value for FeO: 0.0 / (3.0 + 2.0 + 3.0 + 0.0) = 0.0.*

Figure 7: Meredig et al. (2014) Phys. Rev. B89, 094104

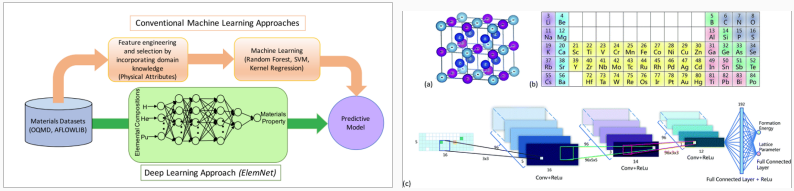


Figure 8: Jha et al. (2018) Sci. Rep., 8(1), 17593., Zheng, X., et al (2018). Chem. Sci., 9(44), 8426-8432.

Structural features

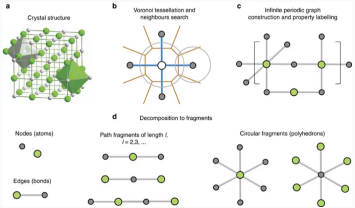


Figure 9: Property-labelled materials fragments + gradient boosting decision tree.[9]

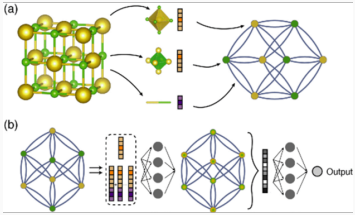


Figure 10: Crystal graph + graph convolutional neural networks

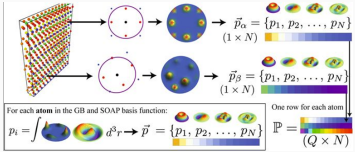


Figure 11: Smooth overlap of atom positions (SOAP).[10]

Example: Graph-based representations

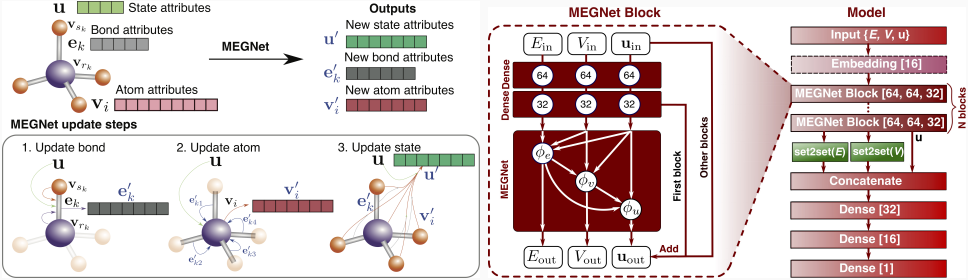


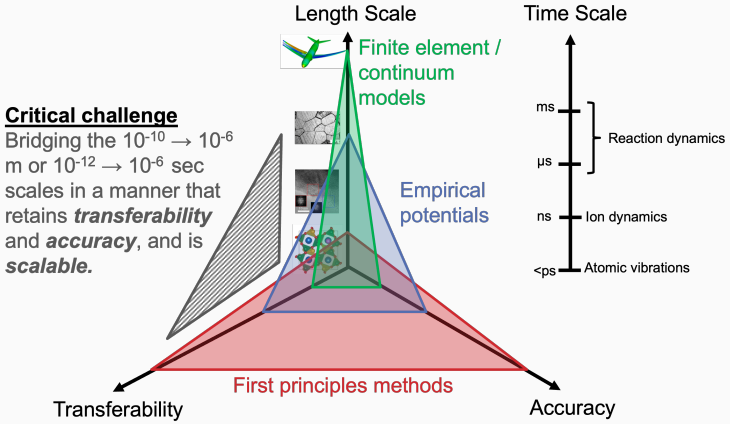
Figure 12: MatErials Graph Networks (MEGNet).[11]

MEGNet Performance Benchmarks

Property	MEGNet	SchNet	CGCNN
Formation energy E_f (meV/atom)	28 (60,000)	35	39 (28,046)
Band gap E_g (eV)	0.330 (36,720)	-	0.388 (16,485)
$\log_{10} K_{VRH}$ (GPa)	0.050 (4,664)	-	0.054 (2,041)
$\log_{10} G_{VRH}$ (GPa)	0.079 (4,664)	-	0.087 (2,041)
Metal classifier	78.9% (55,391)	-	80% (28,046)
Non-metal classifier	90.6% (55,391)	-	95% (28,046)

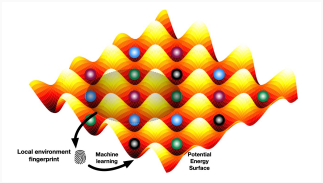
Table 1: Materials Project Crystals. Brackets indicate number of data points.

Scale Challenge in Materials Science



Critical challenge
Bridging the $10^{-10} \rightarrow 10^{-6}$ m or $10^{-12} \rightarrow 10^{-6}$ sec scales in a manner that retains ***transferability*** and ***accuracy***, and is ***scalable.***

ML Interatomic Potentials as a solution to the scale challenge



- Examples: Neural Network Potential (NNP)[12], Gaussian Approximation Potential (GAP)[13], moment tensor potential (MTP)[14], spectral neighbor analysis potential,[15], atomic cluster expansion[16], etc.
- ML models: Linear regression, Gaussian kernels, neural networks, etc.
- Local environment descriptors:

$$G_i^{\mathrm{atom,rad}} = \sum_{j \neq i}^{N_{\mathrm{atom}}} e^{-\eta(R_{ij}-R_s)^2} \cdot f_c(R_{ij}),$$

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

$$\rho_i(\boldsymbol{R}) = \sum_j f_c(R_{ij}) \cdot \exp(-\frac{|\boldsymbol{R}-\boldsymbol{R}_{ij}|^2}{2\sigma_{\mathrm{atom}}^2}),$$

Automatable workflows for MLIP Construction

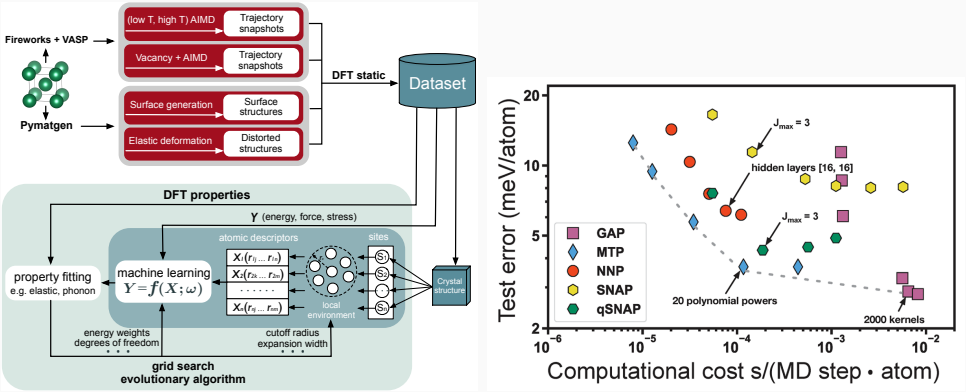


Figure 13: Automatic workflow for ML-IAP construction and performance benchmarks.[17]

Example: Ni-Mo

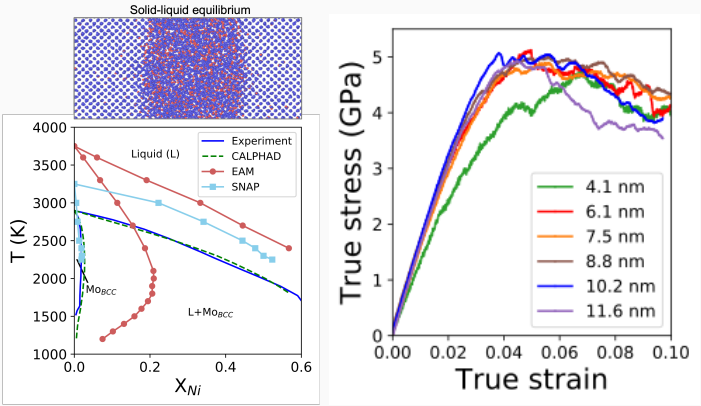


Figure 14: MLIP results on Ni-Mo. (left) Ni-Mo phase diagram. (right) Stress-strain curves as a function of grain size[17]

Universal MLIPs

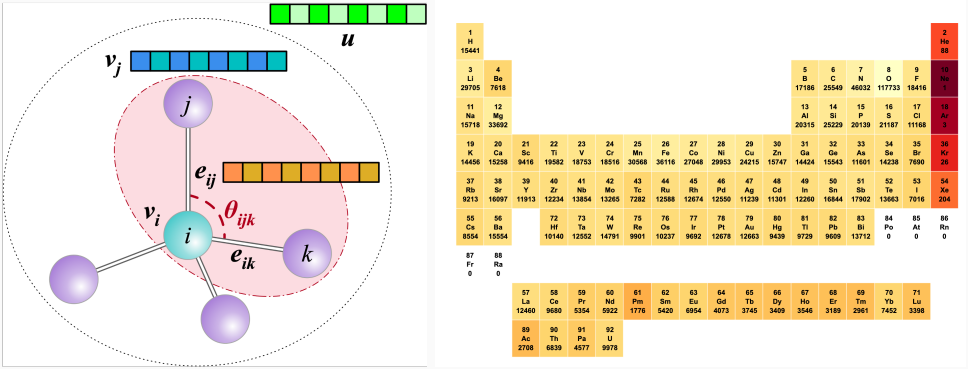


Figure 15: Materials 3-body Graph Network (M3GNet), the first whole periodic table MLIP.[18]

Modeling complex relationships

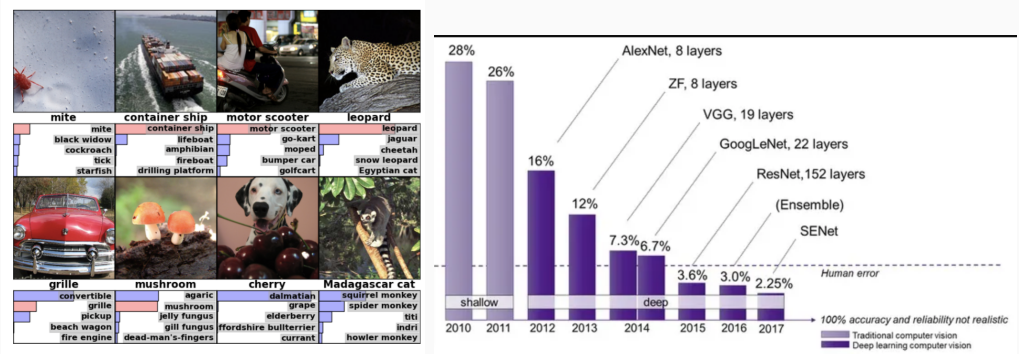
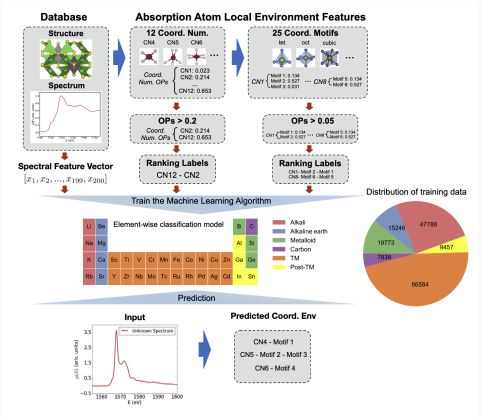


Figure 16: ImageNet (https://www.image-net.org/)

Example: Coordination environment from X-ray Absorption Spectra



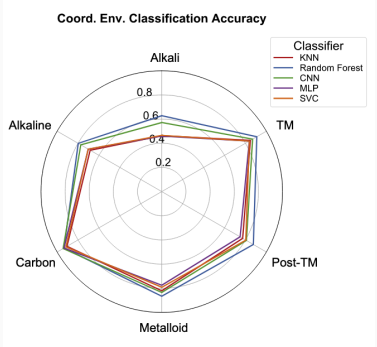


Figure 17: Random Forest Coordination Environment Classification[19]

Other examples

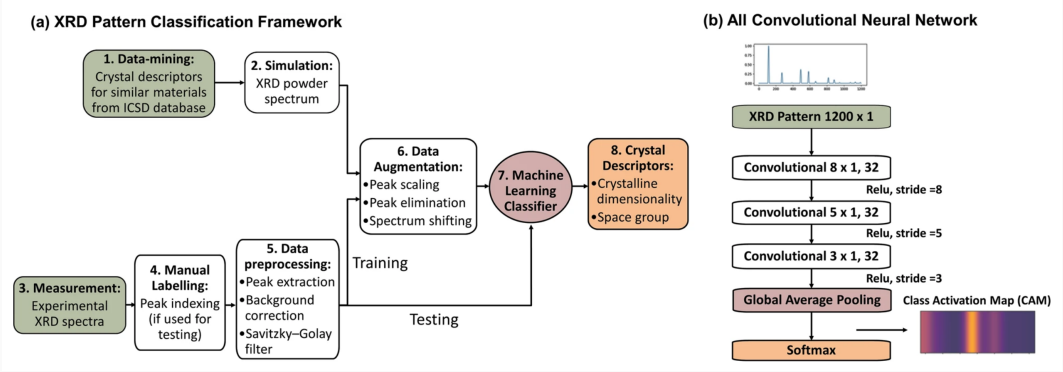


Figure 18: X-ray diffraction data classification with CNNs[20]

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