

# Introduction to Data Science in Materials Science

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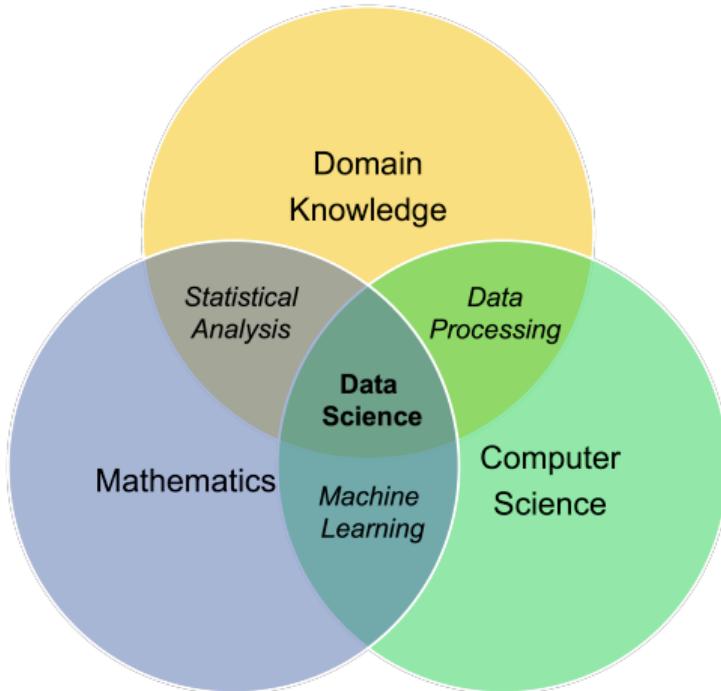
University of California, San Diego

Fall 2023

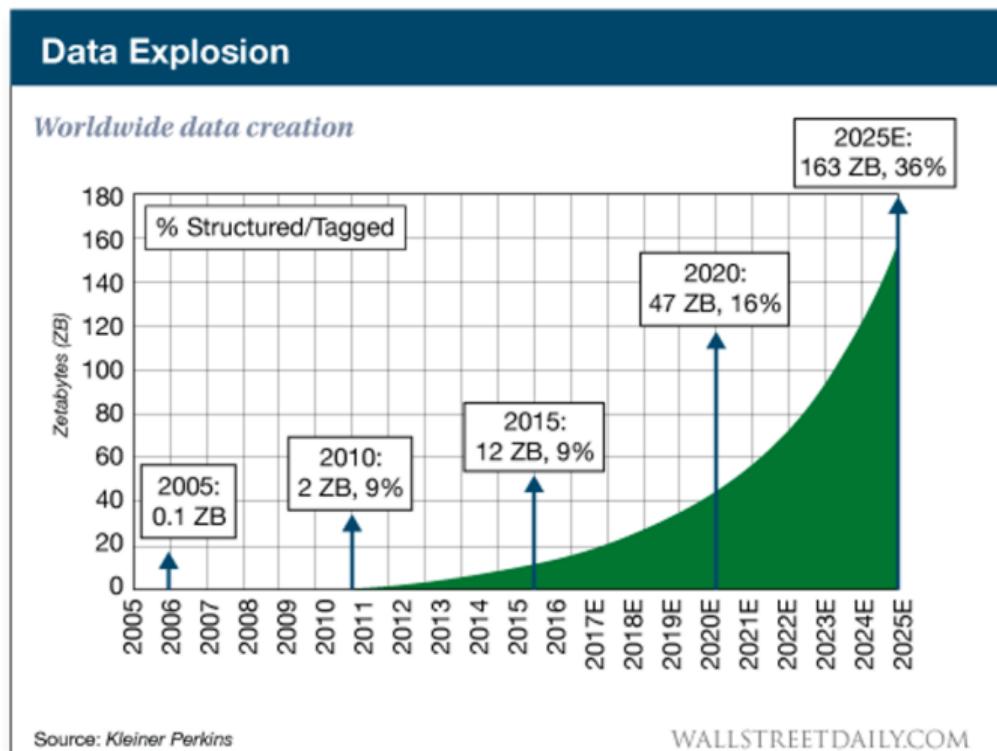
## What is Data Science?

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



# Growth of Materials Data (as of Jan 1 2020)

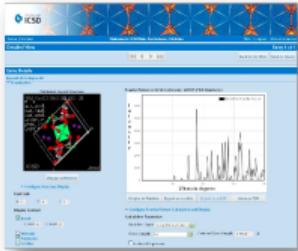


Figure: ICSD: ~200,000 crystals



Figure: COD: ~400,000 crystals

>138,000 STRUCTURES OF PROTEINS, DNA, AND RNA

#### THE PDB ARCHIVE

- Grows at the rate of nearly 10% per year
- Used to download more than 1.8 Million structure data files per day
- Managed by International collaboration US-Australia-Europe
- Manages "Big Data" as global Public Good

#### PDB DATA

- Enable research in subject areas from Agriculture to Zoology
- Contributed data to nearly 1 million published research papers
- Used by >400 biological data resources

Figure: Protein data bank

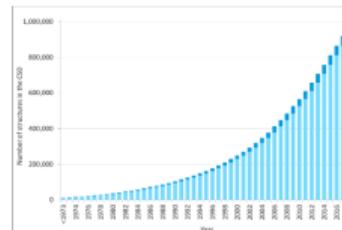
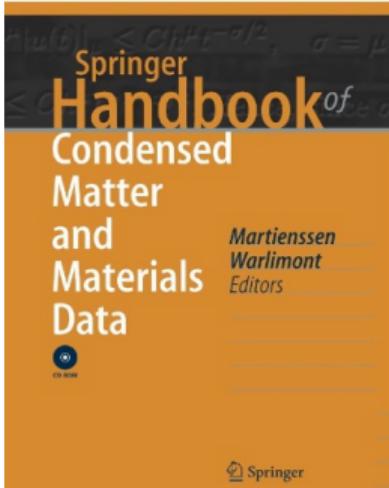


Figure: Cambridge structural database (small-molecule organic crystal structures)  
Fall 2023

# But Quantity and Quality Lags Many Other Fields



**Figure:** 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...

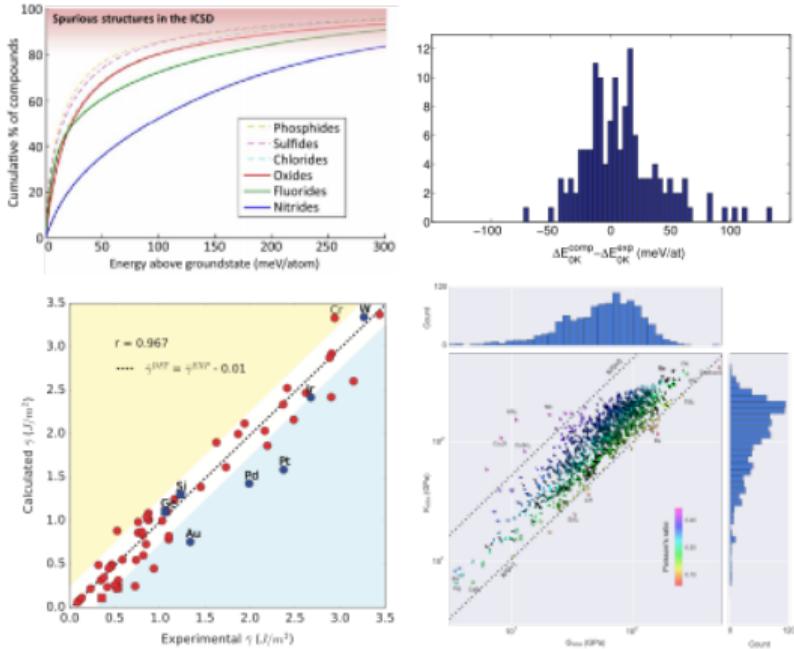
The screenshot shows the SuperCon website. At the top, there is a navigation bar with links for Japanese, For New User, National Institute for Materials Science, Home, About us, MTS Symposium, Link, Contact us, NIMS, and MatNavi. The main header says "Super Con" and "Superconducting Material Database (SuperCon)". On the left, there is a "LOGIN" button and a registration form. The registration form includes fields for "MatNavi" (checkbox), "Free of charge" (checkbox), and "All you need to do is register." Below the form are links for Register, Forget your Password?, Update registration, and Close your account. A "Guest User" link is also present. On the right, there is a section titled "Outline" which describes SUPERCON as a numerical database for superconducting materials. It mentions that all data is acquired from published journals and refers to old data. It also notes two tables: OXIDE &amp; METALLIC (inorganic materials containing metals, alloys compounds, oxide high-Tc superconductors, etc.) and ORGANIC (organic superconductors). Further down, there is information about STA-DB (Standardized Data for Typical Oxide High-Tc materials), INFO-DB (Knowledge data for materials researchers), and a SUMMARY section.

**Figure:** ~1000+ superconductors (many minor composition modifications). Ref:  
<https://supercon.nims.go.jp/>



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

		average $\Delta E$	$\Delta E$
	KLK	0.6	0.3 0.3 0.6 1.0 0.9 0.3
	existing	0.5	0.3 0.1 0.5 0.9 0.8 0.2
	PHI-aims/tier2	0.5	0.3 0.1 0.5 0.9 0.8 0.2
	PLQR	0.6 0.8 0.5 0.5	0.8 0.6 0.4
	FFLO/T4F*	0.9 1.0 0.9 0.9 0.8	0.9 0.9
	RSP	0.8 0.9 0.6 0.6 0.9	0.8
	WEINROCK/acc	0.9 0.3 0.2 0.2 0.4	0.9 0.8
AE	GRV1L/ABINIT	0.9 0.8 0.8 0.9	1.3 1.1 0.8
AE	GPW90S/ABINIT	1.4 1.3 1.3 1.3 1.7 1.5 1.3	
AE	GPW90/GRW	1.6 1.5 1.5 1.5 1.8 1.7 1.5	
AE	JTH02/ABINIT	0.6 0.6 0.6 0.6 0.9 0.7 0.5	
PAW	PSSLR00/QE	0.9 0.8 0.8 0.8	1.3 1.1 0.8
PAW	VASP/HG2015/VASP	0.6 0.4 0.4 0.6 1.0 0.8 0.3	
PAW	GRV14/CASTEP	1.1 1.1 1.1 1.0 1.4 1.3 1.0	
PAW	GRV14/QE	1.1 1.0 0.9 1.0 1.4 1.3 1.0	
PAW	OTFGS/CASTEP	0.7 0.6 0.5 0.5 1.0 1.0 0.5	
PAW	SSSEF/QE	0.5 0.4 0.3 0.5 0.9 0.8 0.3	
PAW	Vib2/CASTEP	6.3 6.3 6.3 6.3 6.4 6.5 6.2	
USPP	PH19pp/ABINIT	13.1 13.1 13.4 13.4 13.2 13.0 13.2 13.4	
USPP	HNL-HNLCC/WigglePPT	2.1 2.2 2.2 2.2 2.0 2.3 2.2 2.1	
USPP	HNL-HNLCC/WigglePPT	1.1 1.1 1.1 1.1 1.0 1.2 1.1 1.0	
USPP	HKR2015/sepIMX	2.0 2.1 2.3 2.3 1.9 1.8 1.8 2.0	
USPP	ONCVPSP (POO-11)/ABINIT	0.7 0.7 0.7 0.6 1.0 0.8 0.6	
USPP	ONCVPSP (SGG15)1/QE	1.4 1.4 1.3 1.3 1.3 1.6 1.5 1.3	
USPP	ONCVPSP (GGG15)2/CASTEP	1.4 1.4 1.4 1.4 1.3 1.6 1.5 1.4	



- (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,[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

The image displays three separate web interfaces for scientific databases:

- OQMD:** The Open Quantum Materials Database. The header includes a navigation bar with Home, Materials, Analysis, Documentation, and Download. A banner at the top says "Newsflash: OQMD v1.1 is out! (Download it [here](#).)".
- AFLOW:** Automatic - FLOW for Materials Discovery. The header includes a navigation bar with HOME, CONSORTIUM, PUBLICATIONS, and SEARCH.
- The Materials Project**: A dark-themed interface featuring geometric shapes and a hexagonal grid background. It highlights "Harnessing computation to accelerate materials discovery" and displays "Database Statistics" with the following counts:

Database Statistics			
124,515	52,827	35,336	530,243
INORGANIC COMPOUNDS	BANDSTRUCTURES	MOLECULES	NANOPOROUS MATERIALS
13,751	3,016	4,401	16,128
ELASTIC TENSORS	PIEZOELECTRIC TENSORS	INTERCALATION ELECTRODES	CONVERSION ELECTRODES

Below these screenshots is a horizontal navigation bar with links: REPOSITORY HOME, REPOSITORY TEAM, WHY SHARING?, DOIs, TERMS, FAQ, UPLOAD YOUR FILES, SEARCH AND DOWNLOAD, and CONTACT US.

**THE NOMAD REPOSITORY**

The NOMAD Repository was established to host, organize, and share materials data.

# Google for Materials

## Materials Genome Initiative: A Renaissance of American Manufacturing

June 2011: **Materials Genome Initiative** which aims to “**fund computational tools, software, new methods for material characterization, and the development of open standards and databases that will make the process of discovery and development of advanced materials faster, less expensive, and more predictable**”

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### First-Of-Its-Kind Search Engine Will Speed Materials Research

November 8, 2011 - 11:05am

Washington, D.C. – Researchers from the Department of Energy's (DOE's) Lawrence Berkeley National Laboratory (Berkeley Lab) and the Massachusetts Institute of Technology (MIT) jointly launched today a groundbreaking new online tool called the Materials Project, which operates like a “Google” of material properties, enabling scientists and engineers from universities, national laboratories and private industry to accelerate the development of new materials, including critical materials.

“By accelerating the development of new materials, we can drive discoveries that not only help power clean energy, but also are used in common consumer products,” said Secretary of Energy Steven Chu. “This research tool will help the United States compete with other developers of new materials, and could potentially create new domestic industries.”

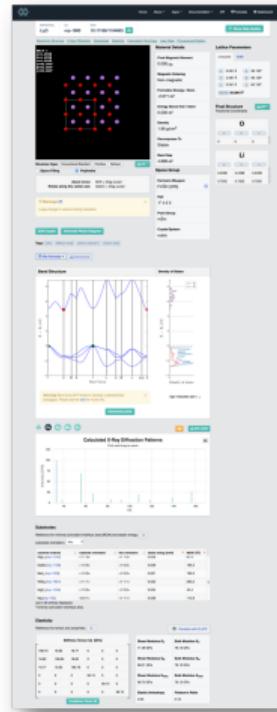
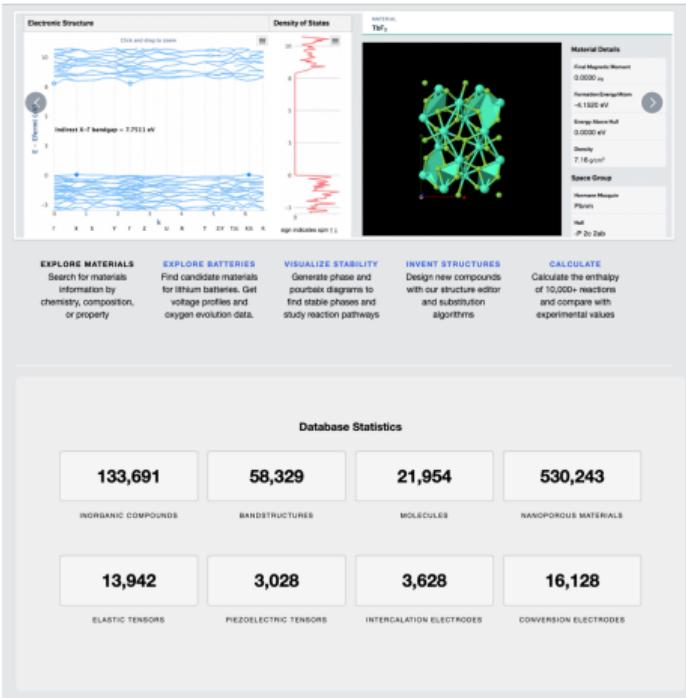
Discovering new materials and strengthening the properties of existing materials are key to improving energy efficiency and fuel use. From building insulation to wind turbine blades, advances in a great variety of materials (“designer materials”) are more important to America’s competitiveness than ever before – particularly in the clean energy field. Cell phones, wind turbines, solar panels and a variety of military technologies depend on these roughly fourteen elements (including now “rare earth” elements). With about 90 percent coming from China, there are growing concerns about potential supply shortages and disruptions.

With the Materials Project, researchers can use supercomputers to characterize properties of



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

Example response:

```
{  
    "data": [  
        {"_id": "61a2dcaa2c86325a0218b5ef", "formation_energy_per_atom": -1.6299189062500006},  
        {"_id": "61a2dcbb52c86325a021af9bd", "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.
- 

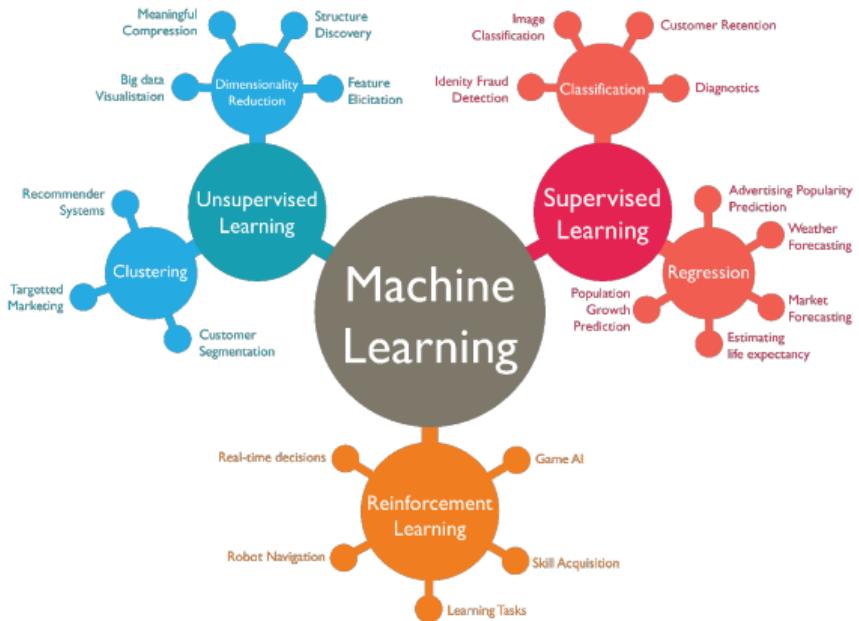
## Ranked data

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

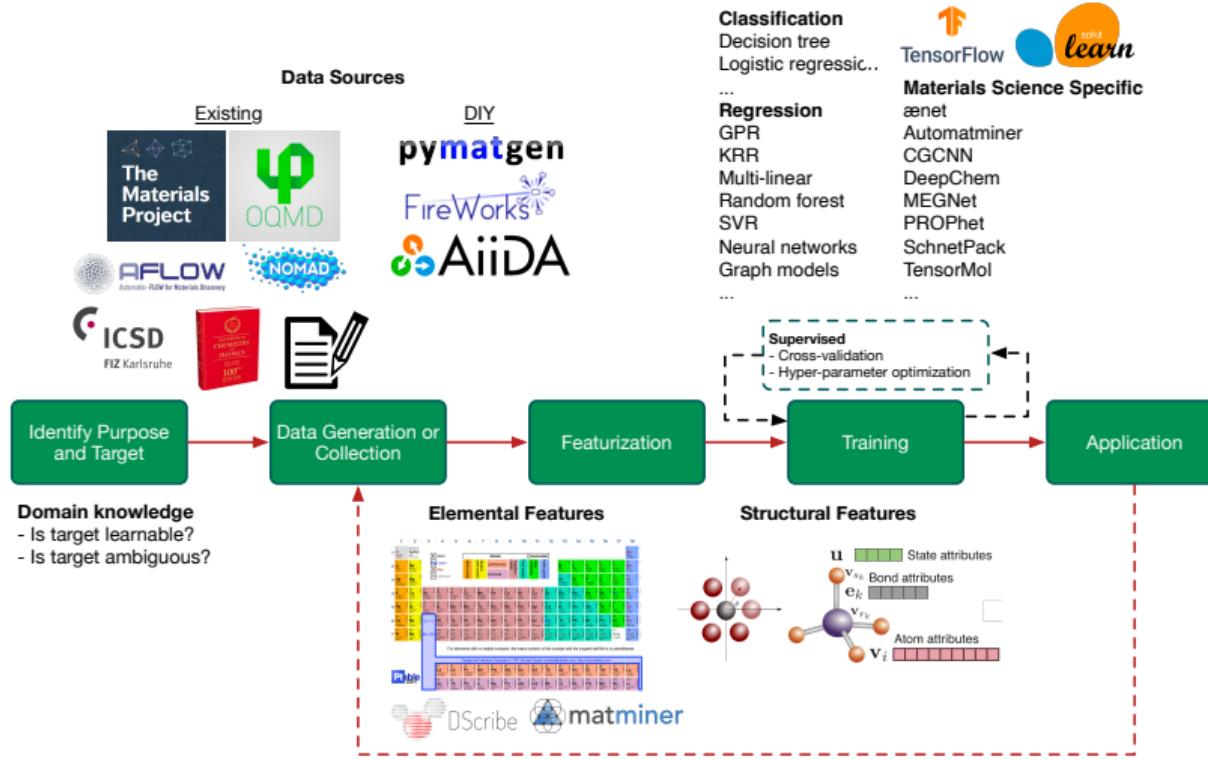
## Quantitative Data

- 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?

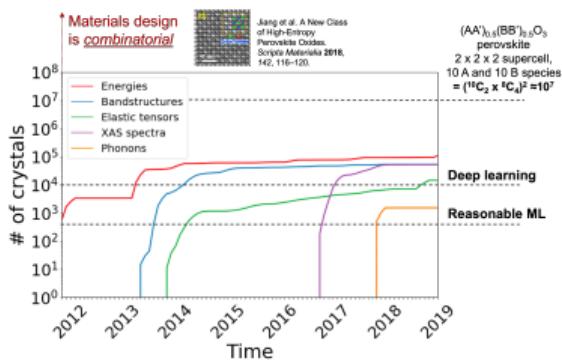


# Materials ML Workflow

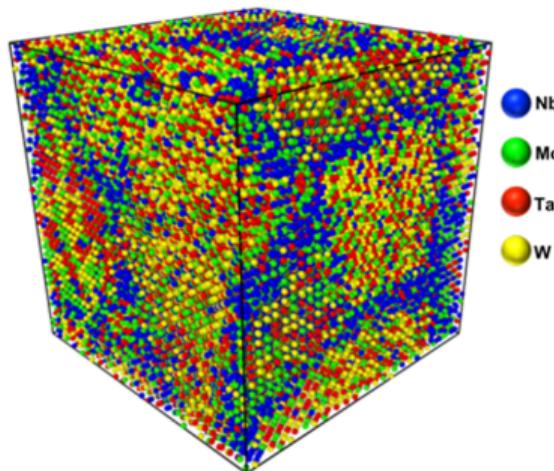


# Where is ML valuable in Materials Science?

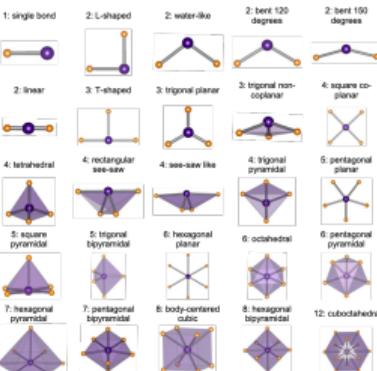
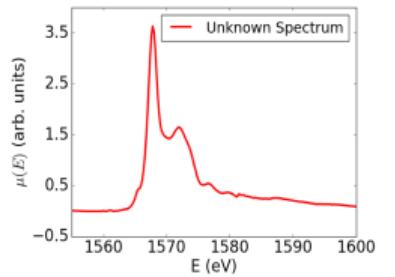
Too many to compute



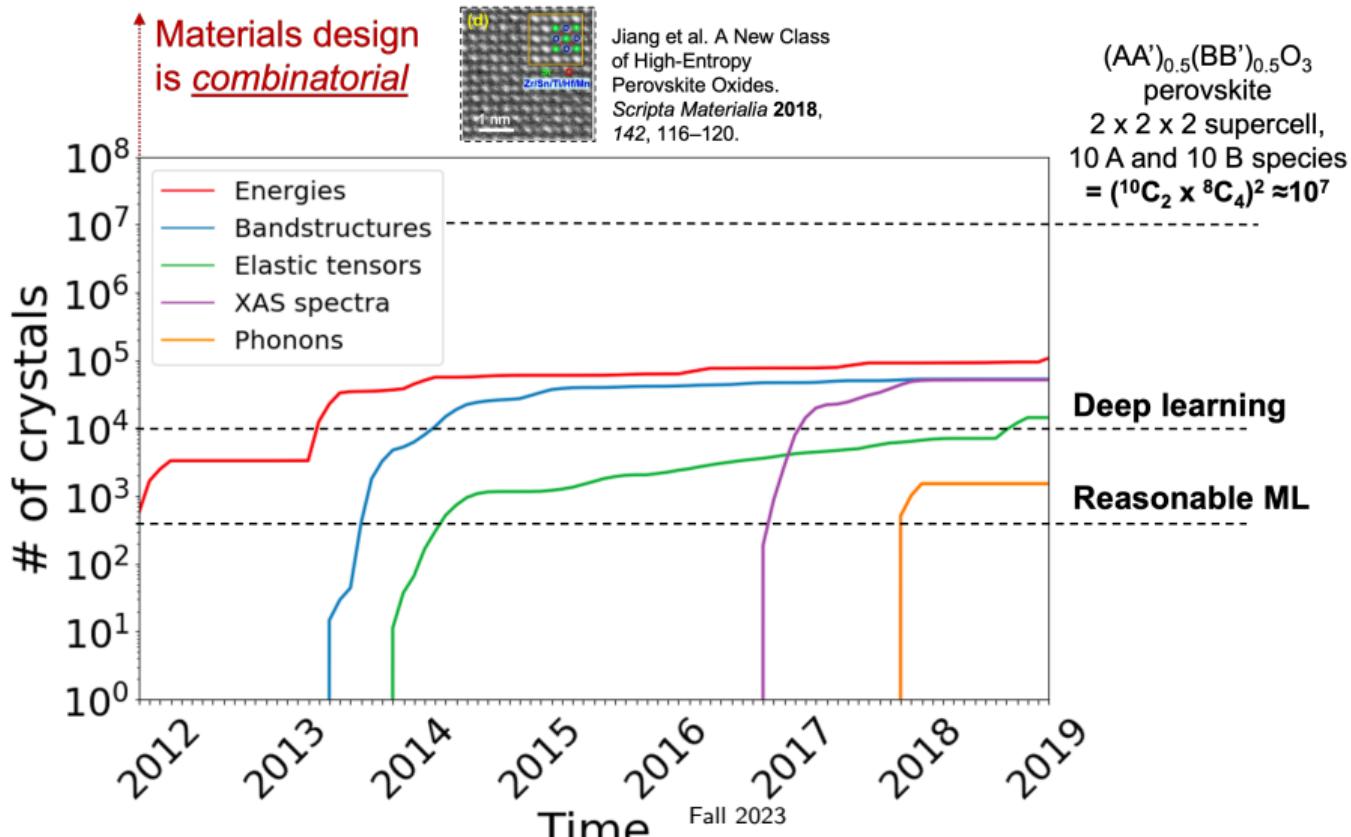
Too big to compute



Too complex to understand.



# Data History of the Materials Project



# Surrogate models for “instant” property predictions

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

- In ML terms, the material property, e.g., energetic (formation, energy above hull, reaction, binding, 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 compositional features: stoichiometric attributes, e.g., number and ratio of elements, etc. elemental properties, e.g., mean, range, min, max of atomic number, electronegativity, row, group, atomic radii, etc., electronic structure, e.g., number of valence electrons, shells, 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:  $0.5 \times 55.845 + 0.5 \times 15.999 = 35.92$ .
- Average column on periodic table:** Composition-weighted average of the columns of the elements in the compound. Value for FeO:  $0.5 \times 8 + 0.5 \times 16 = 12.0$ .
- Average row on the periodic table:** Composition-weighted average of the rows of the elements in the compound. Value for FeO:  $0.5 \times 4 + 0.5 \times 2 = 3.0$ .
- 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:  $0.5 \times 26 + 0.5 \times 8 = 17.0$ .
- 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:  $0.5 \times 140 + 0.5 \times 60 = 100.0$ .
- 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:  $0.5 \times 3.44 + 0.5 \times 1.83 = 2.635$ .
- 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:  $0.5 \times 4 + 0.5 \times 2 = 3.0$ .
- Average number of p valence electrons:** Analogous to above, but for p electrons. Value for FeO:  $0.5 \times 0 + 0.5 \times 6 = 2.0$ .
- Average number of d valence electrons:** Analogous to above, but for d electrons. Value for FeO:  $0.5 \times 6 + 0.5 \times 0 = 3.0$ .
- Average number of f valence electrons:** Analogous to above, but for f electrons. Value for FeO:  $0.5 \times 0 + 0.5 \times 0 = 0.0$ .
- 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:  $0.0 / (3.0 + 2.0 + 3.0 + 0.0) = 0.0$ .

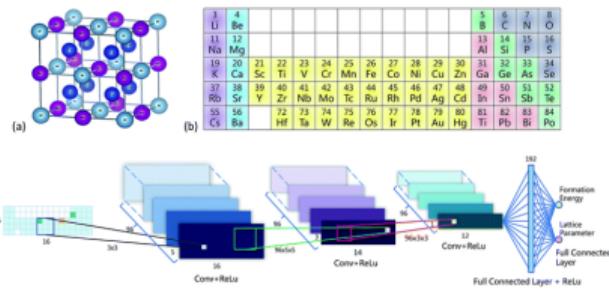
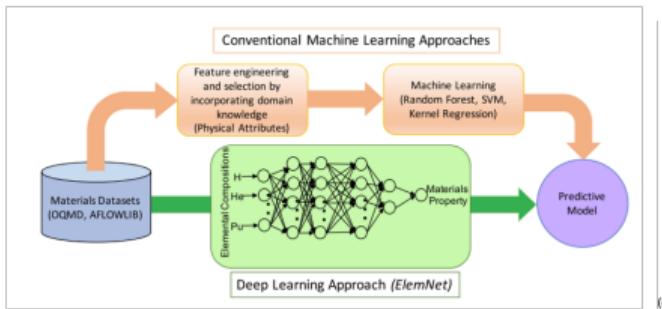


Figure: Jha et al. (2018) Sci. Rep., 8(1), 17593., Zheng, X., et al (2018). Chem. Sci., 9(44), 8426-8432.

Figure: Meredig et al. (2014) Phys. Rev. B89, 094104  
NANOx81

# Structural features

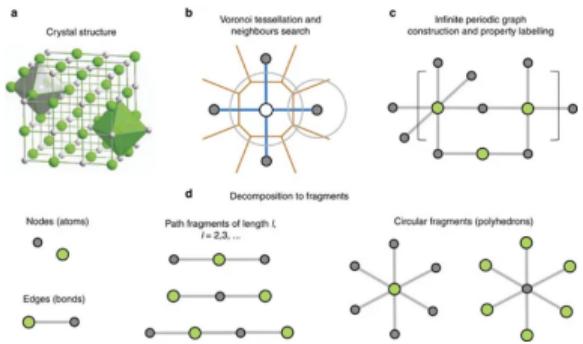


Figure: Property-labelled materials fragments + gradient boosting decision tree.[9]

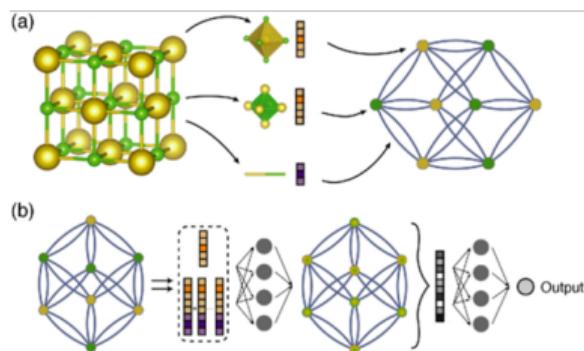


Figure: Crystal graph + graph convolutional neural networks

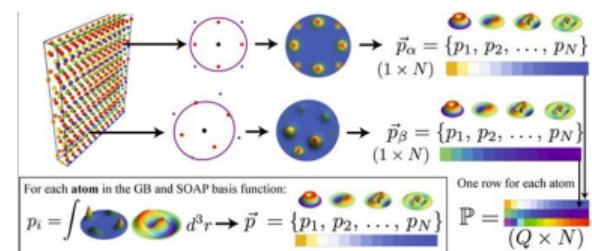


Figure: Smooth overlap of atom positions (SOAP).[10]

# Example: Graph-based representations

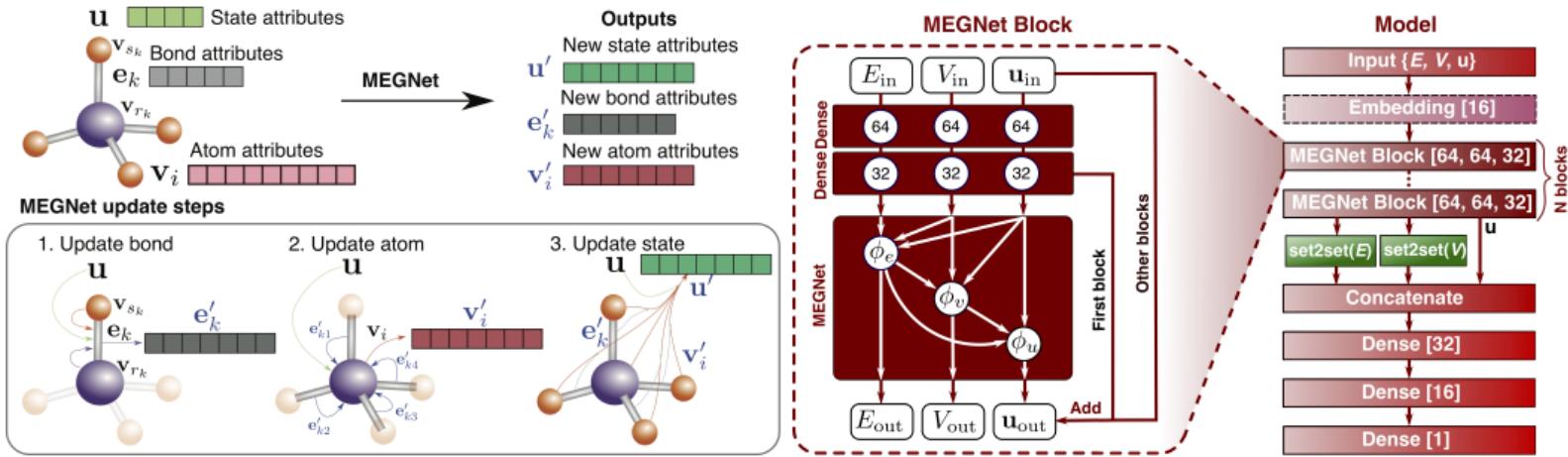


Figure: MatErials Graph Networks (MEGNet).[11]

# MEGNet Performance Benchmarks

	MEGNET	MEGNET-Simple	SchNet	"Chemical Accuracy"
U <sub>0</sub> (meV)	9	12	14	43
G (meV)	10	12	14	43
$\varepsilon_{HOMO}$ (eV)	0.038	0.043	0.041	0.043
$\varepsilon_{LUMO}$ (eV)	0.031	0.044	0.034	0.043
C <sub>v</sub> (cal/molK)	0.030	0.029	0.033	0.05

Table: 130,462 QM9 molecules

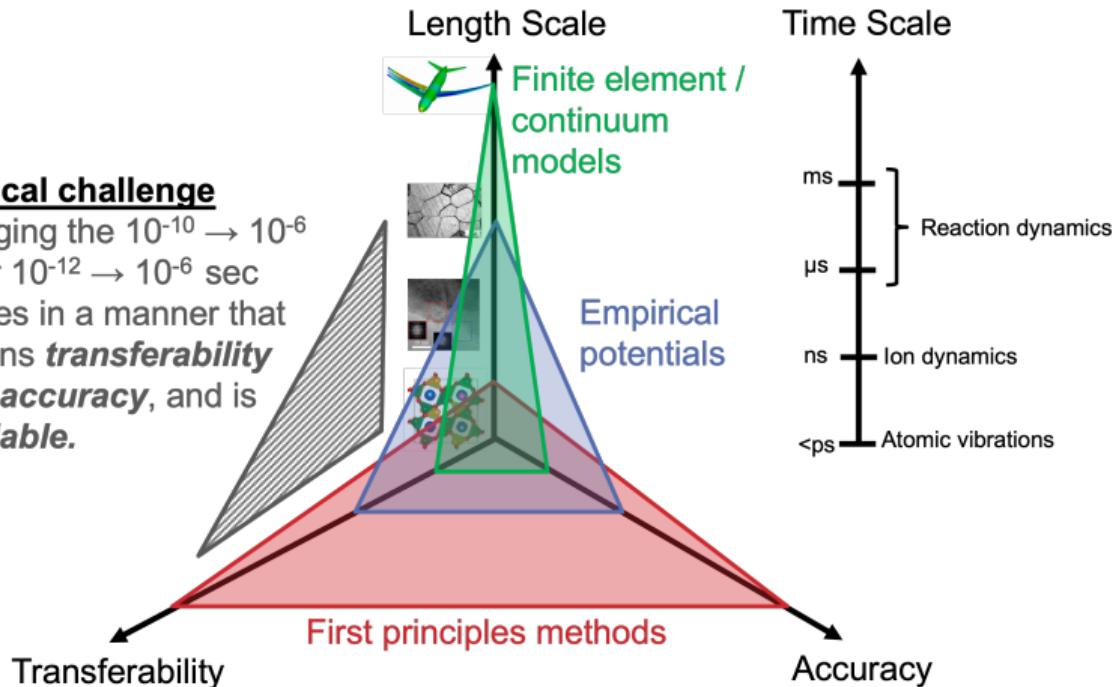
Property	MEGNet	SchNet	CGCNN
Formation energy $E_f$ (meV/atom)	28 (60,000)	35	39 (28,046)
Band gap $E_g$ (eV)	0.330 (36,720)	-	0.388 (16,485)
$\log_{10} K_{VRH}$ (GPa)	0.050 (4,664)	-	0.054 (2,041)
$\log_{10} G_{VRH}$ (GPa)	0.079 (4,664)	-	0.087 (2,041)
Metal classifier	78.9% (55,391)	-	80% (28,046)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

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

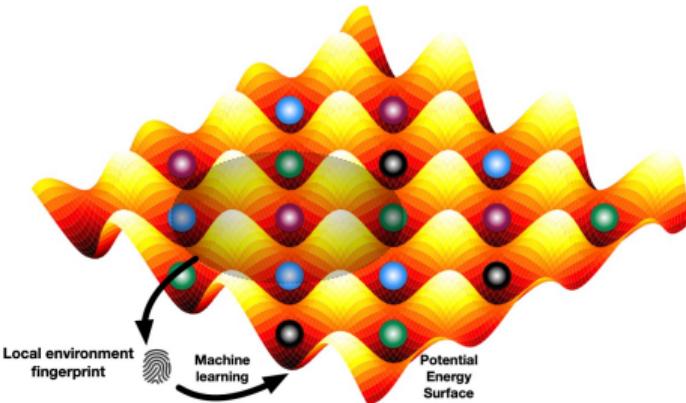
# Scale Challenge in Materials Science

## 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 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:

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

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

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

# Automatable workflows for ML Interatomic Potential Construction

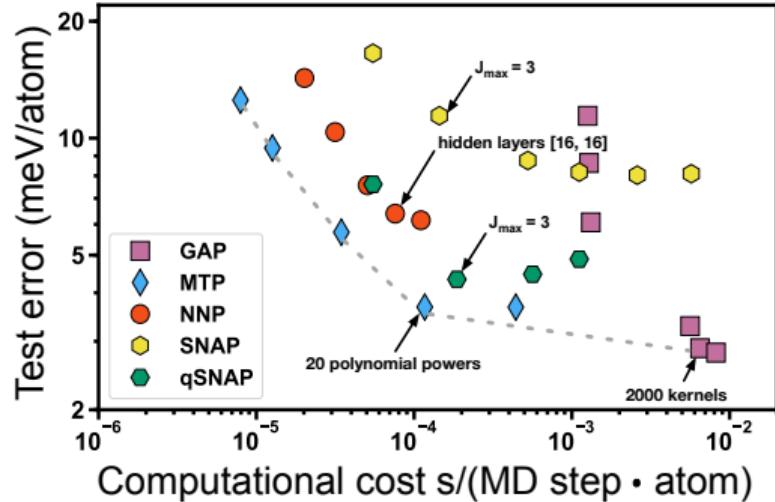
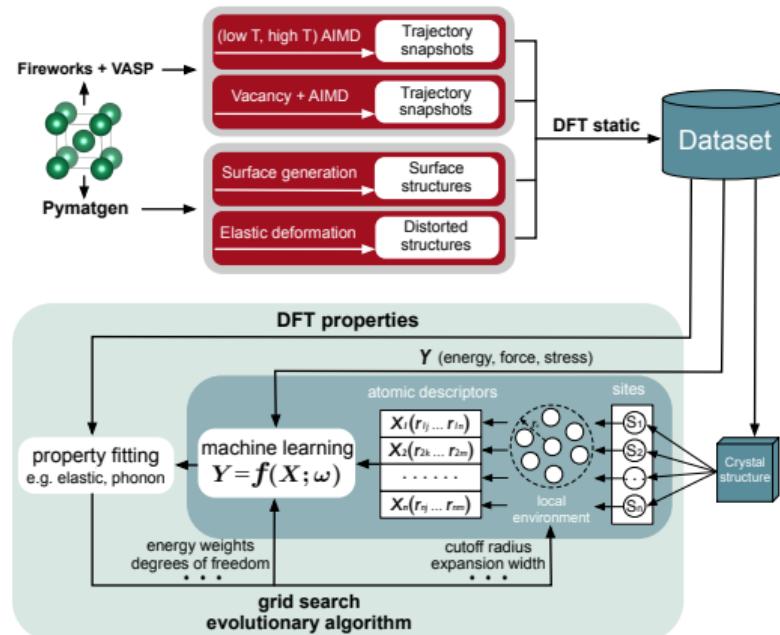


Figure: Automatic workflow for ML-IAP construction and performance benchmarks.[17]

## Example: Ni-Mo

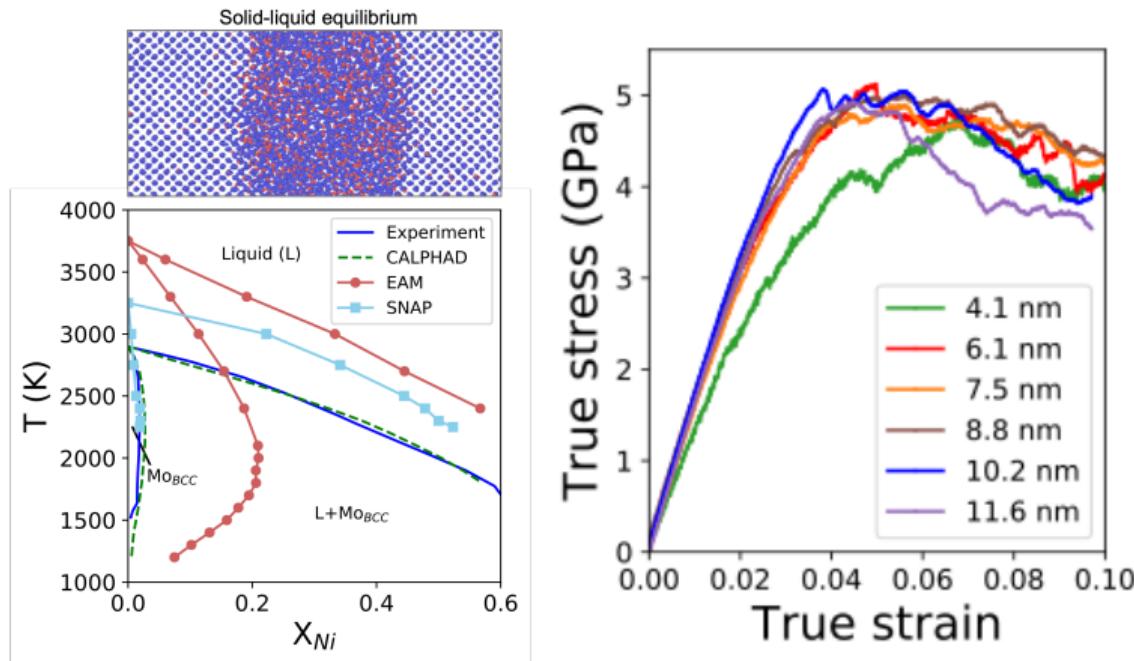


Figure: ML-IAP results on Ni-Mo. (left) Ni-Mo phase diagram. (right) Stress-strain curves as a function of grain size[17]

# Modelling complex relationships

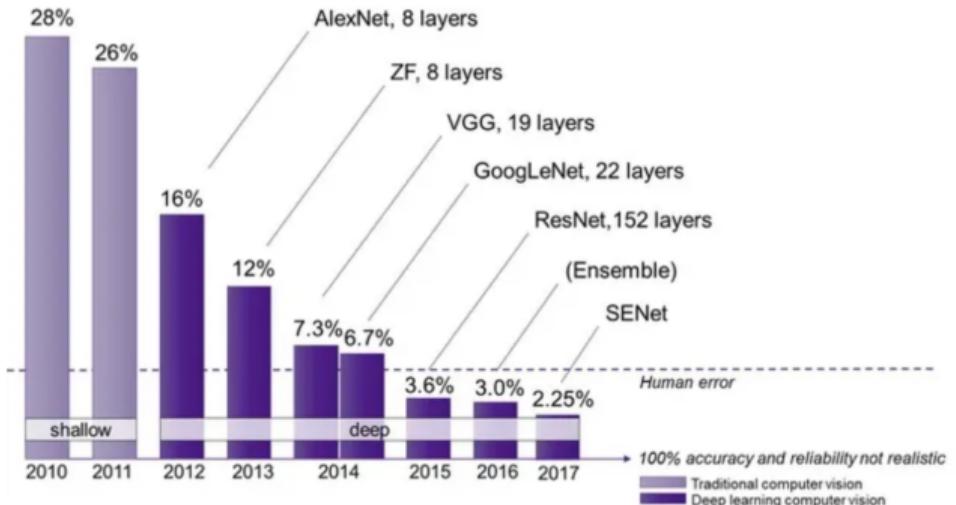
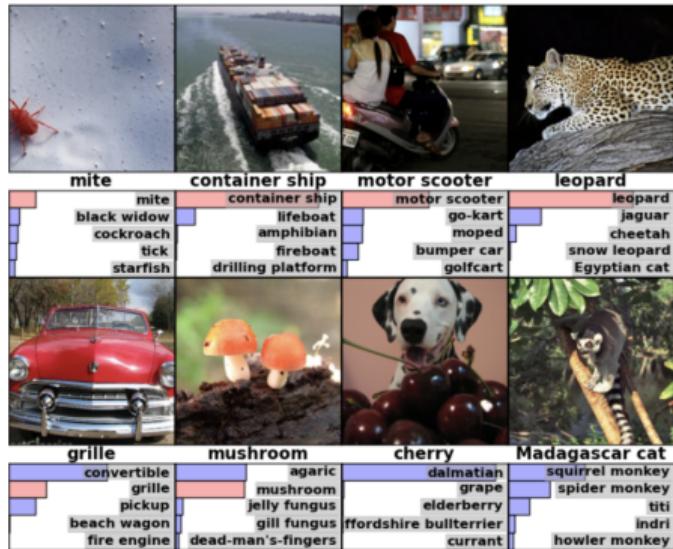
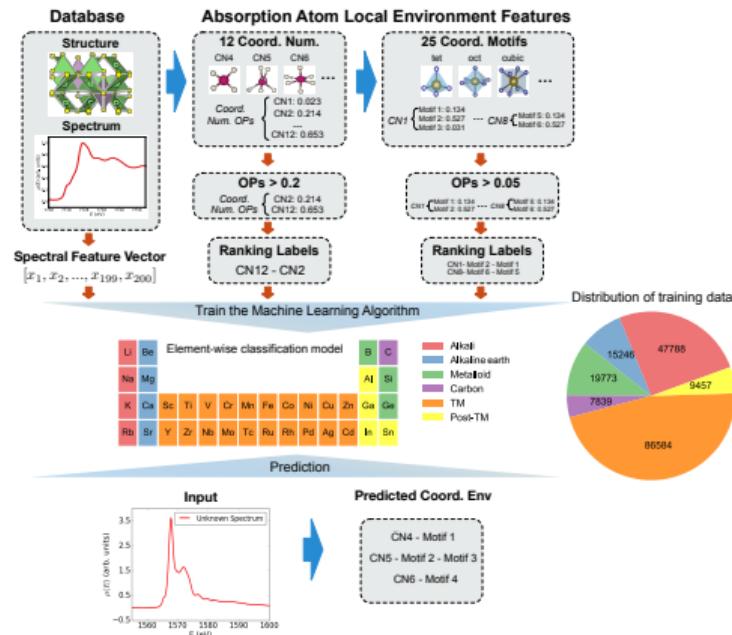


Figure: ImageNet (<https://www.image-net.org/>)

# Example: Coordination environment from X-ray Absorption Spectra



Coord. Env. Classification Accuracy

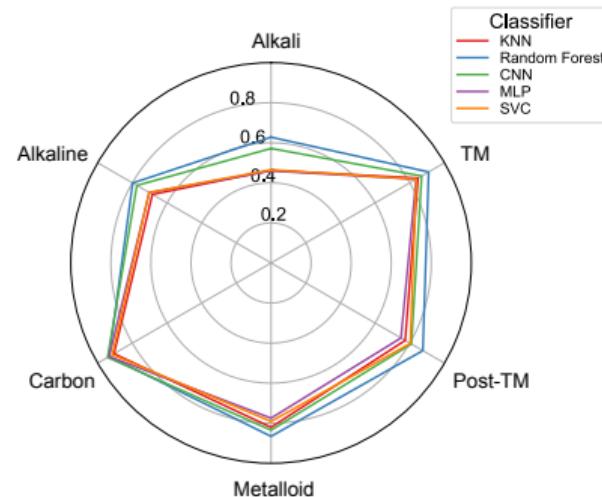
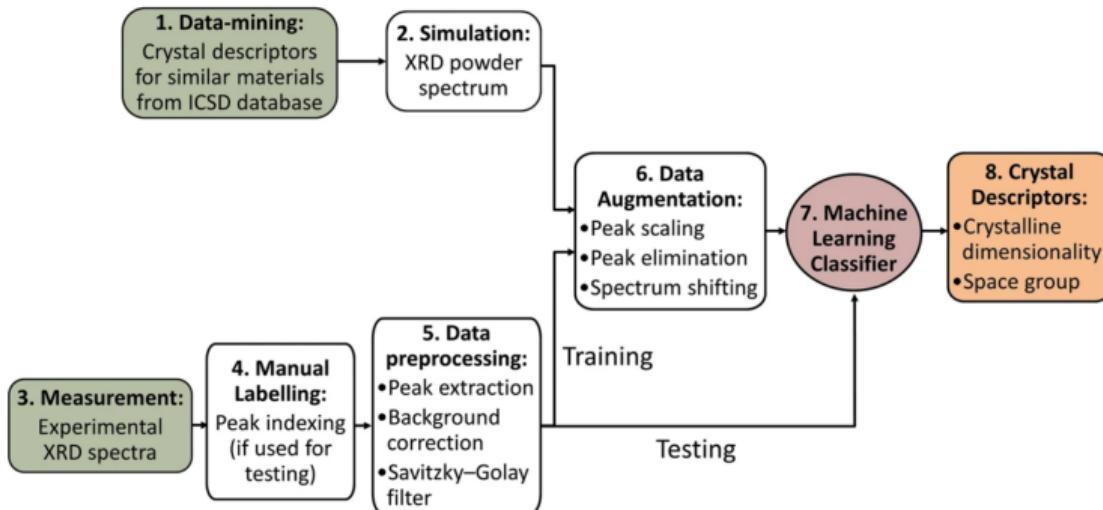


Figure: Random Forest Coordination Environment Classification[18]

# Other examples

(a) XRD Pattern Classification Framework



(b) All Convolutional Neural Network

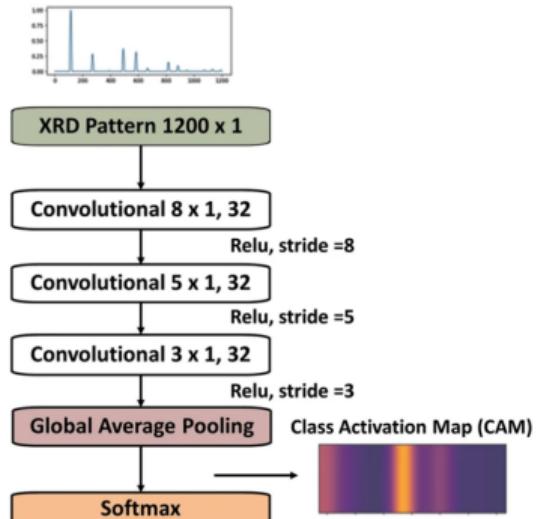


Figure: X-ray diffraction data classification with CNNs[19]

# Bibliography I

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