

Introduction to Data Science in Materials Science

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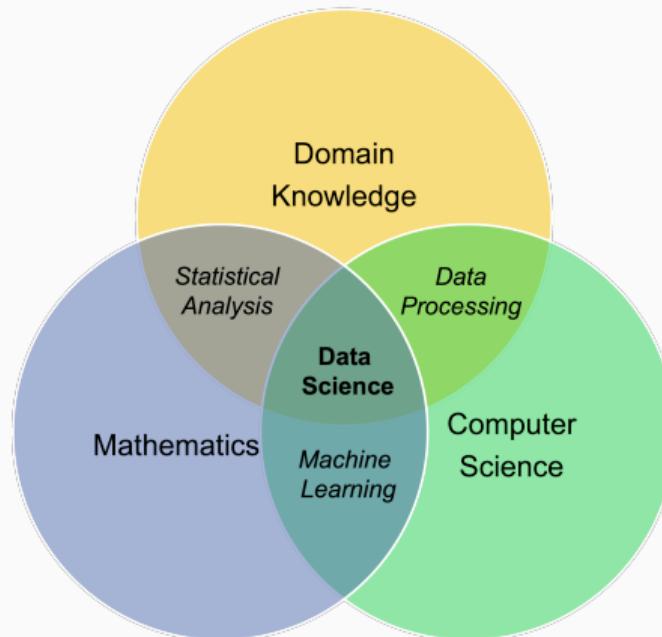
University of California, San Diego

<http://materialsvirtuallab.org>

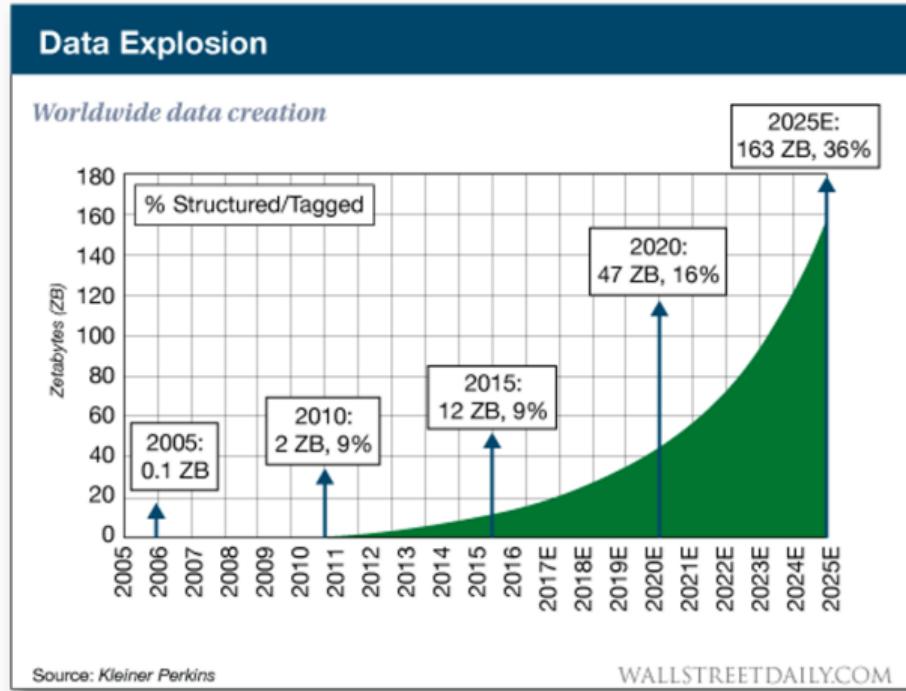
What is Data Science?

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 in Materials Data (as of Jan 1 2020)

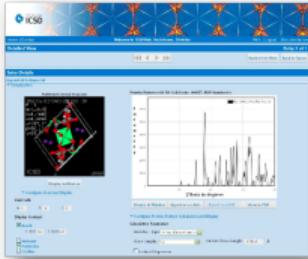


Figure 1: ICSD: ~200,000 crystals



Figure 2: COD: ~400,000 crystals

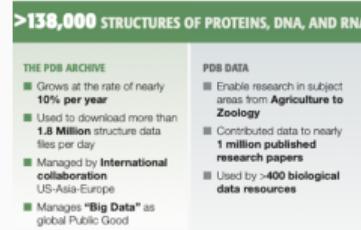


Figure 3: Protein data bank

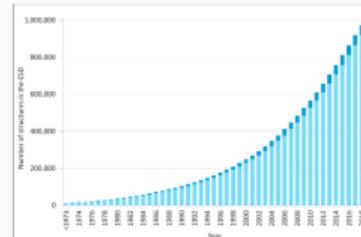


Figure 4: Cambridge structural database (small-molecule organic crystal structures)

But Quantity and Quality Lags Many Other Fields

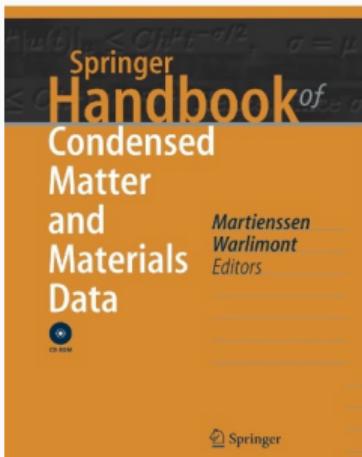
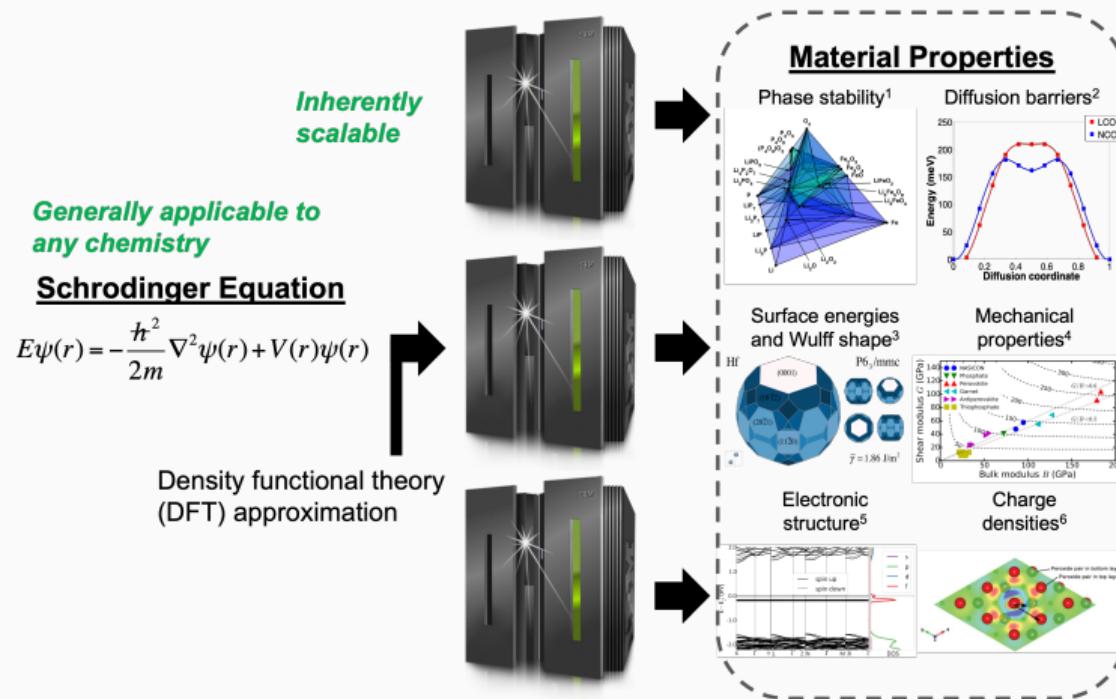


Figure 5: One of the most comprehensive handbooks on materials data: Density, thermal and electrical conductivity, melting and boiling points, etc., but O(100) binaries and limited ternaries...

The screenshot displays the homepage of the SuperCon website. At the top, there's a navigation bar with links for Japanese, For New User, National Institute for Materials Science, Home, About us, MITS Symposium, Link, Contact us, NIMS, and MatNet. The main content area is titled "Superconducting Material Database (SuperCon)". It features a "LOGIN" section with a checkbox for "The use of 'MatNet' is free. (Free of charge)" and several registration links. Below this is an "Outline" section with a brief description of the database. Further down are sections for "STA-DB (Standardized Data for Typical Oxide High-Tc materials)", "INFO-DB (Knowledge data for materials researchers)", and a "SUMMARY" section. The entire page has a clean, modern design with green and white color scheme.

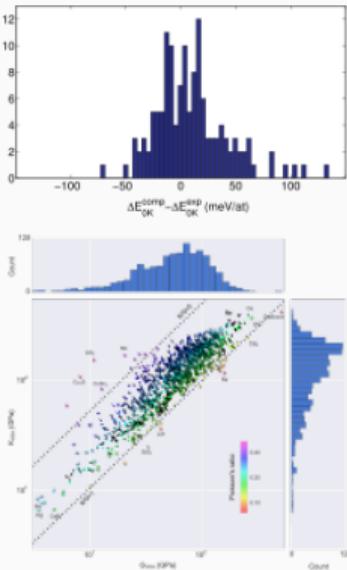
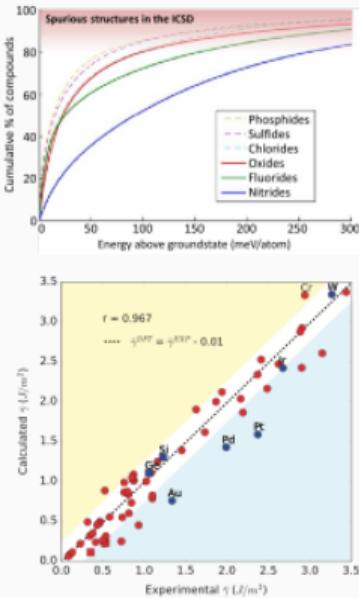
Figure 6: ~1000+ superconductors (many minor composition modifications). Ref: <https://supercon.nims.go.jp/>

First Principles Materials Computations



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

	AE															
	average <15>		KLB		WILL		PEL-AICAR/TAU2		FIMR		PEO/TYPER*		ASPE		WIMERS/Aspe	
KLB	0.6		0.3	0.3	0.6	1.0	0.9	0.3								
maxline	0.5	0.3	0.1	0.1	0.5	0.9	0.8	0.2								
PEO+AIMS/TAU2	0.5	0.3	0.1	0.1	0.5	0.9	0.8	0.2								
FIMR	0.6	0.6	0.5	0.5	0.8	0.8	0.6	0.4								
PEO/TYPER*	0.9	1.1	0.9	0.9	0.8	0.9	0.9	0.9								
ASPE	0.8	0.8	0.8	0.8	0.6	0.9	0.8	0.8								
WIMERS/Aspe	0.5	0.3	0.2	0.2	0.4	0.4	0.3	0.8								
GRHY2/AMRNET	0.9	1.0	0.8	0.8	1.3	1.1	1.0	0.8								
GPW99/AMRNET	1.4	1.3	1.3	1.3	1.3	1.7	1.5	1.3								
GRH99/GRW99	1.6	1.5	1.5	1.5	1.8	1.7	1.5	1.5								
JTH02/AMRNET	0.6	0.6	0.6	0.6	0.6	0.9	0.7	0.5								
PEL-AICAR/TAU2	0.9	0.8	0.8	0.8	0.8	1.3	1.1	0.8								
VASP/POSS/VASP	0.6	0.4	0.4	0.4	0.6	1.0	0.8	0.3								
GRHY4/CASEFF	1.3	1.1	1.1	1.0	1.0	1.4	1.3	1.0								
GRHV14/VASP	1.3	1.0	0.9	1.0	1.4	1.3	1.0	0.9								
OTFGN/CASEFF	0.7	0.4	0.5	0.5	0.7	1.0	1.0	0.5								
SEBP/QE	0.5	0.4	0.3	0.3	0.5	0.9	0.8	0.3								
VASPH/DMC99P	6.3	6.3	6.3	6.3	6.3	6.4	6.5	6.2								
PR19pp/AMRNET	11.3	13.5	13.4	13.4	13.2	13.0	13.2	13.4								
HOM/AMRNET	2.2	2.2	2.2	2.2	2.0	2.3	2.2	2.1								
HOM-HLCC/HOM99P	1.3	1.1	1.1	1.1	1.0	1.2	1.1	1.0								
MM2153/OpenMM	20.1	21.1	21.1	21.1	19.1	18.1	18.1	18.1								
ONCVPPM(DDO_11)/AMRNET	0.7	0.7	0.7	0.7	0.6	1.0	0.8	0.6								
ONCVPPM(1815)/VASP	1.4	1.4	1.3	1.3	1.3	1.6	1.5	1.3								
ONCVPPM(8G15)2/CASEFF	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 screenshots of scientific databases, each with a distinct header and footer.

- OQMD:** The Open Quantum Materials Database. Header: Home, Materials, Analysis, Documentation, Download. Newsflash: OQMD v1.1 is out! (Download it [here](#).)
- AFLW**: Automatic - FLOW for Materials Discovery. Header: HOME, CONSORTIUM, PUBLICATIONS, SEARCH.
- The Materials Project**. Header: Harnessing the power of computation to enable materials innovation. Sub-section: INORGANIC COMPOUNDS (124,515), BANDSTRUCTURES (52,827), MOLECULES (35,336), NANOPOROUS MATERIALS (530,243). Sub-section: ELASTIC TENSORS (13,751), PIEZOELECTRIC TENSORS (3,016), INTERCALATION ELECTRODES (4,401), CONVERSION ELECTRODES (16,128).

REPOSITORY HOME REPOSITORY TEAM WHY SHARING? DOIs TERMS FAQ UPLOAD YOUR FILES SEARCH AND DOWNLOAD 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**”

Subscribe



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

November 3, 2011 – 11:00pm

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 vital in ensuring consumer products," said Secretary of Energy Steven Chu. "The research tool will help the United States compete with other developers of new materials, and could potentially create new domestic industries."

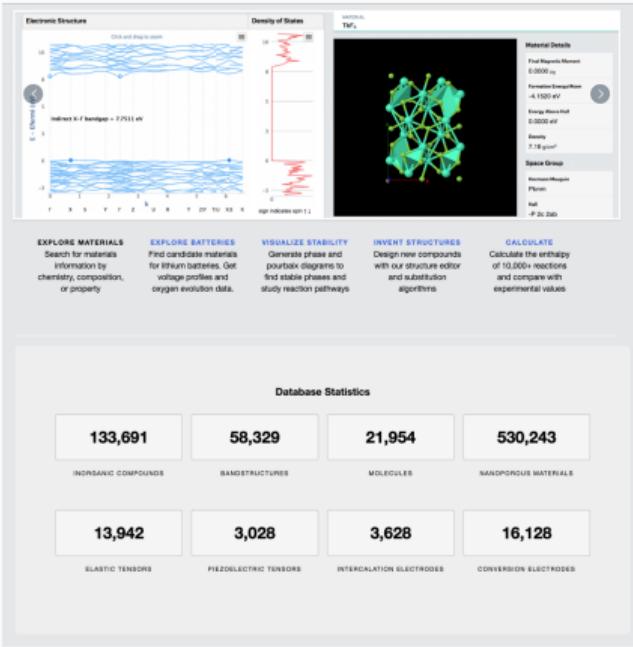
Discovering new materials and strengthening the properties of existing materials are key to improving just about everything humans use – from computers and high-end medical diagnostics, to everyday advances in a variety of materials, like "inert" materials that are important to America's competitiveness 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

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.

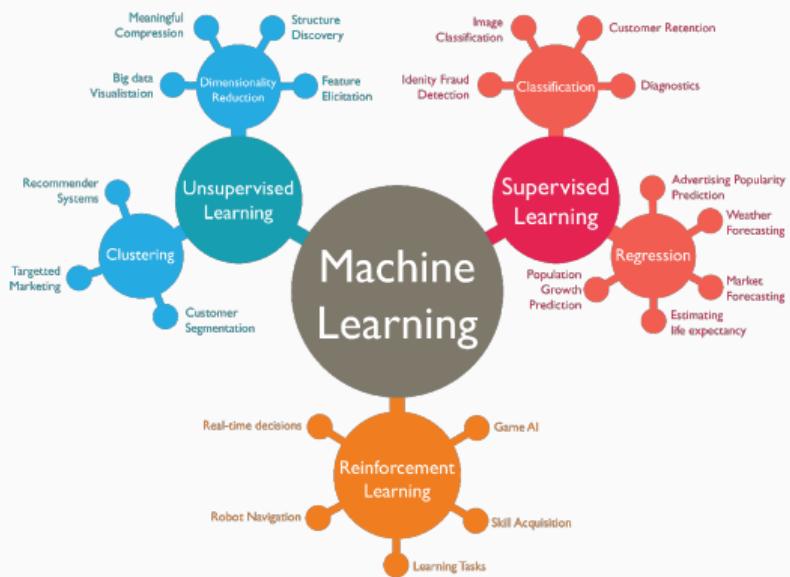
Ranked data

- 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?



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

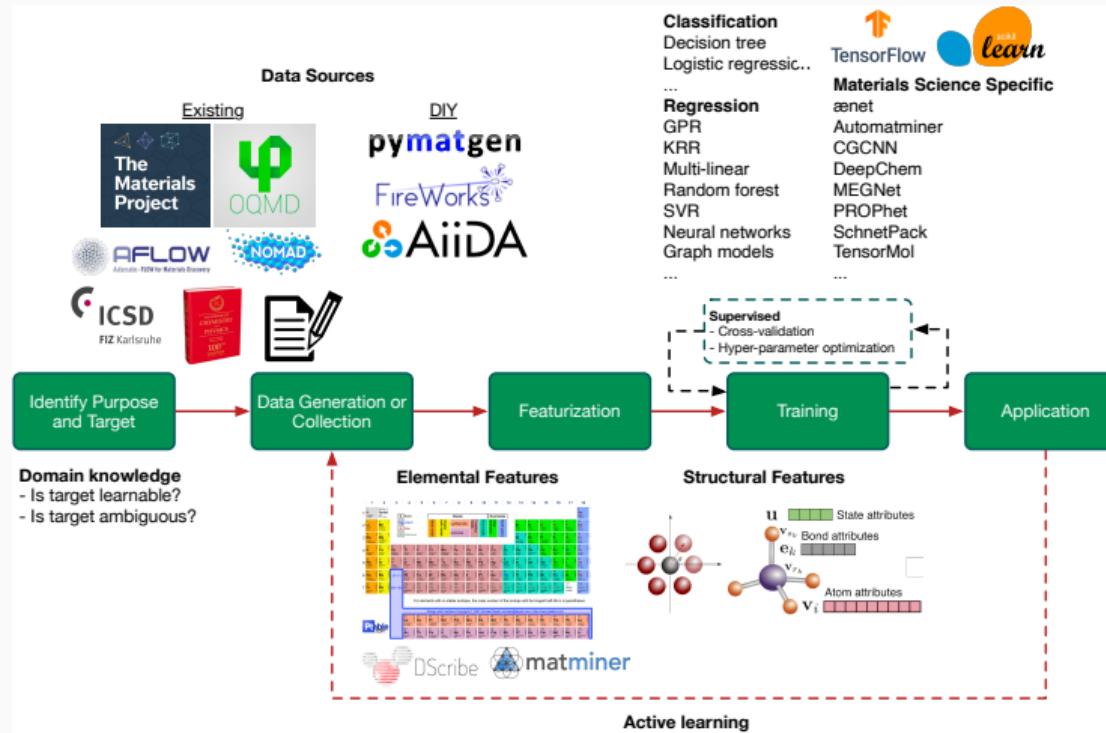
Geoffrey Hinton

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



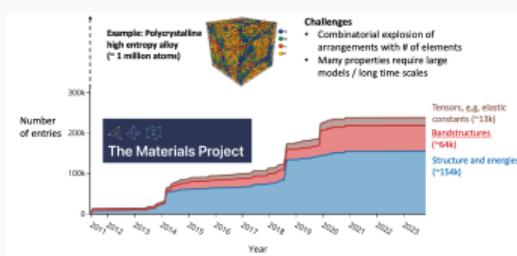
Geoffrey Hinton. Ill. Niklas Elmehed © Nobel Prize Outreach

Materials ML Workflow

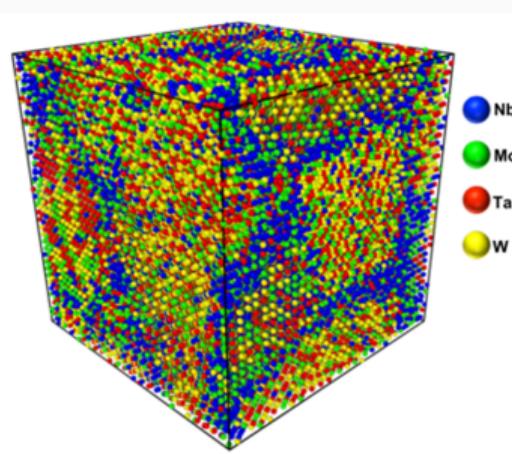


Where is ML valuable in Materials Science?

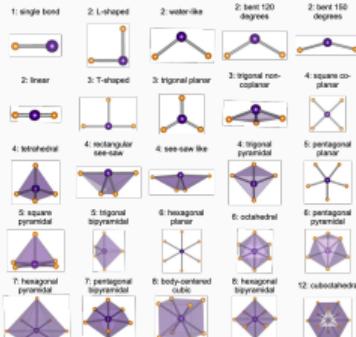
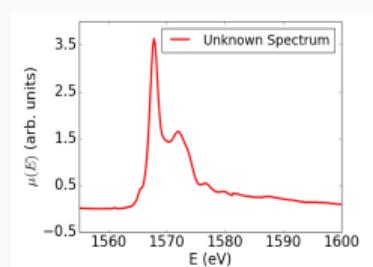
Too many to compute



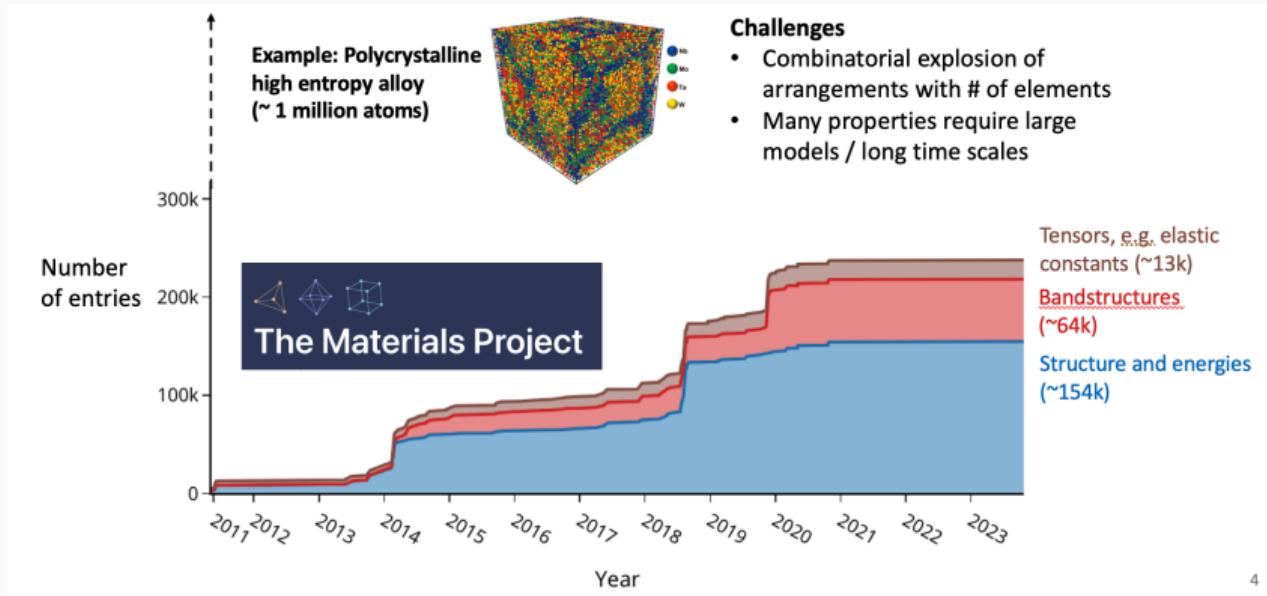
Too big to compute



Too complex to understand.



Data History of the Materials Project



4

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 compositional 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: $0.5 \times 55.845 + 0.5 \times 15.999 = 35.92$.
- 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: $0.5 \times 6 + 0.5 \times 4 = 2.0$.
- Average number of d valence electrons: Analogous to above, but for d electrons. Value for FeO: $0.5 \times 5 + 0.5 \times 0 = 3.0$.
- 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: $0.0 / (3.0 + 2.0 + 3.0 + 0.0) = 0.0$.

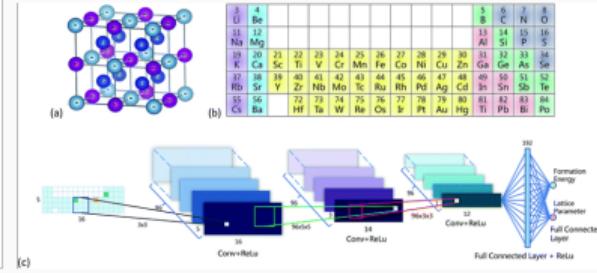
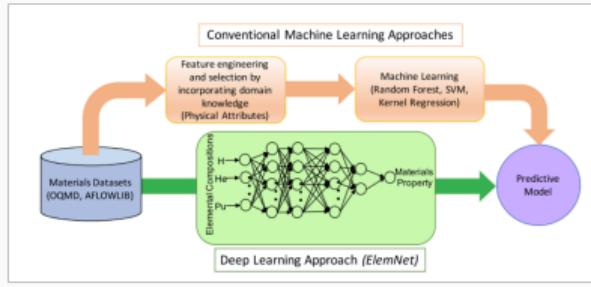


Figure 8: Jha et al. (2018) Sci. Rep., 8(1), 17593., Zheng, X., et al (2018). Chem. Sci., 9(44), 8426-8432.

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

Structural features

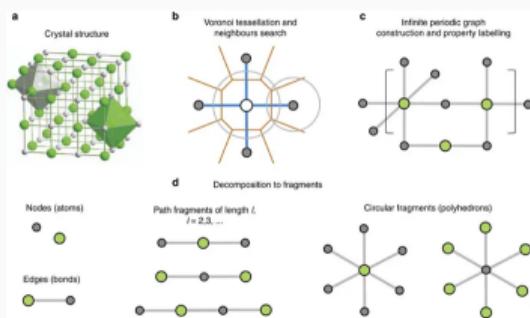


Figure 9: Property-labelled materials fragments + gradient boosting decision tree.[9]

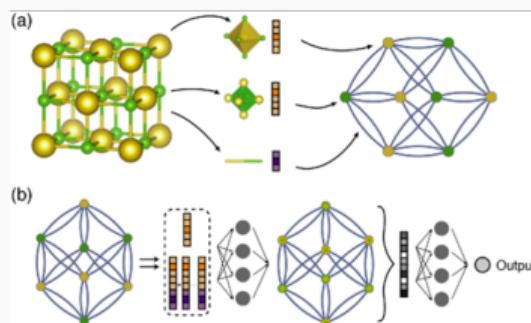


Figure 10: Crystal graph + graph convolutional neural networks

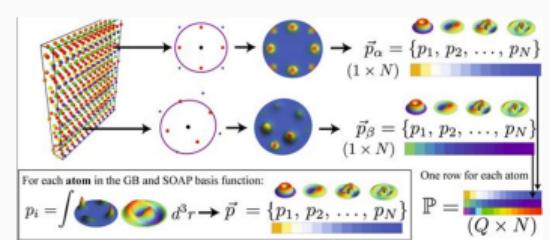


Figure 11: Smooth overlap of atom positions (SOAP).[10]

Example: Graph-based representations

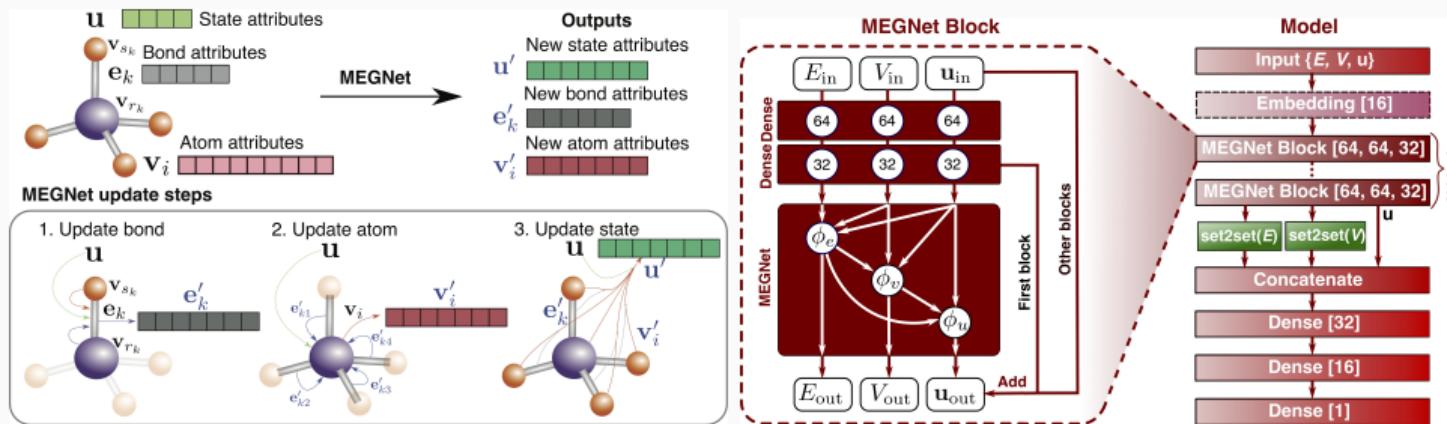


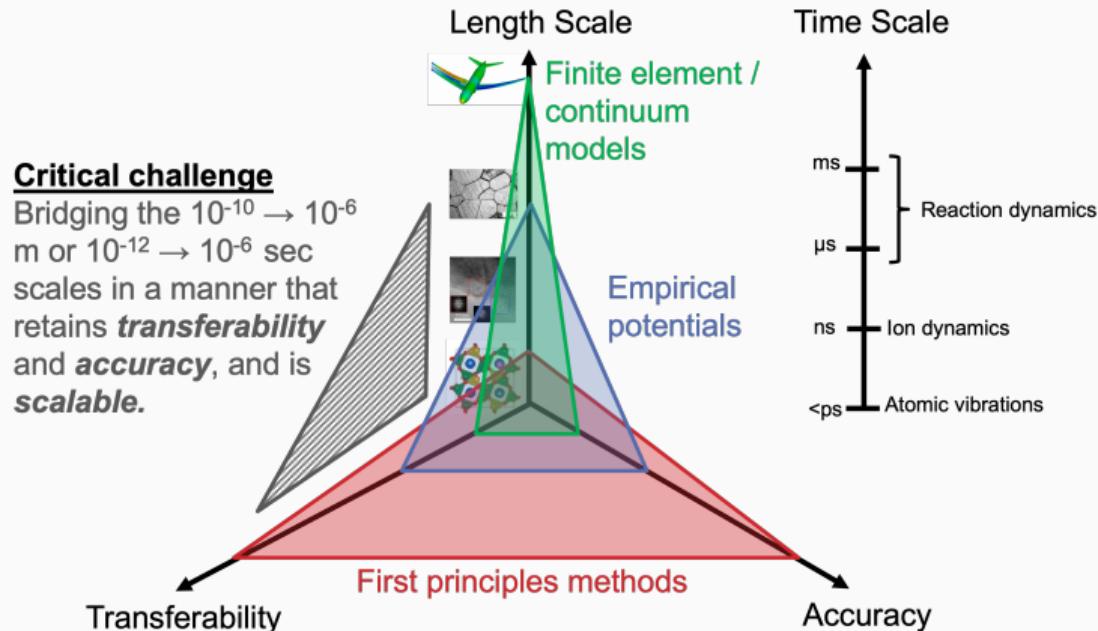
Figure 12: MatErials Graph Networks (MEGNet).[11]

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)

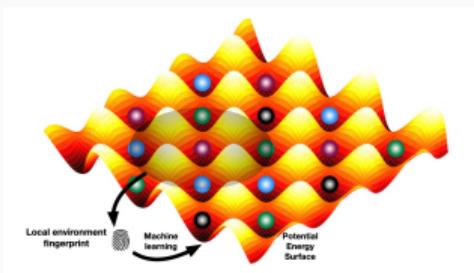
Table 1: Materials Project Crystals. Brackets indicate number of data points.

Scale Challenge in Materials Science



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:



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

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

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

Automatable workflows for MLIP Construction

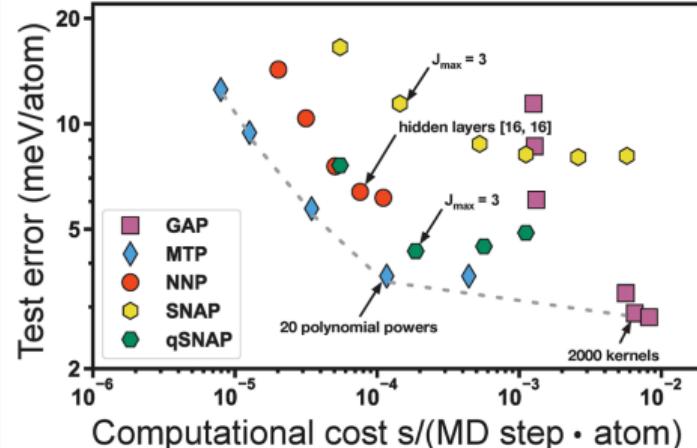
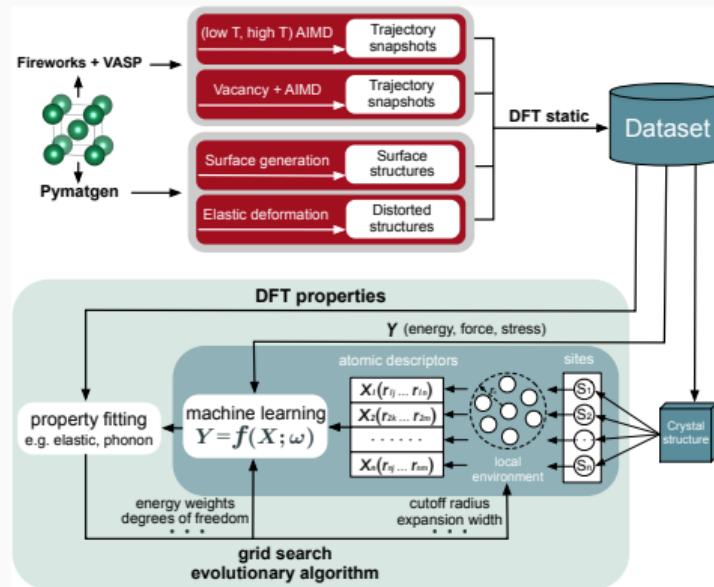


Figure 13: Automatic workflow for ML-IAP construction and performance benchmarks.[17]

Example: Ni-Mo

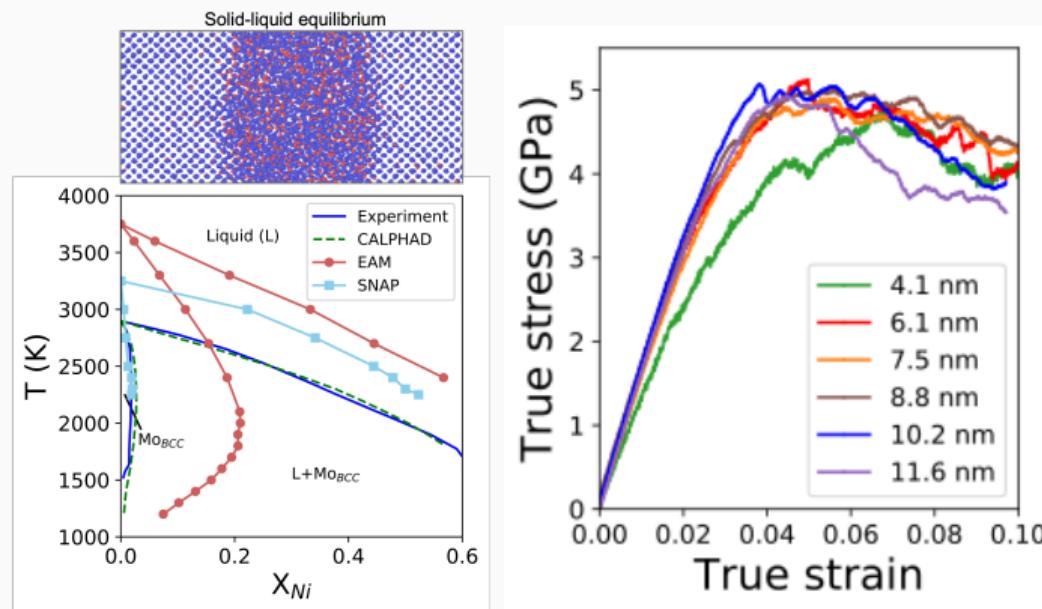


Figure 14: MLIP results on Ni-Mo. (left) Ni-Mo phase diagram. (right) Stress-strain curves as a function of grain size[17]

Universal MLIPs

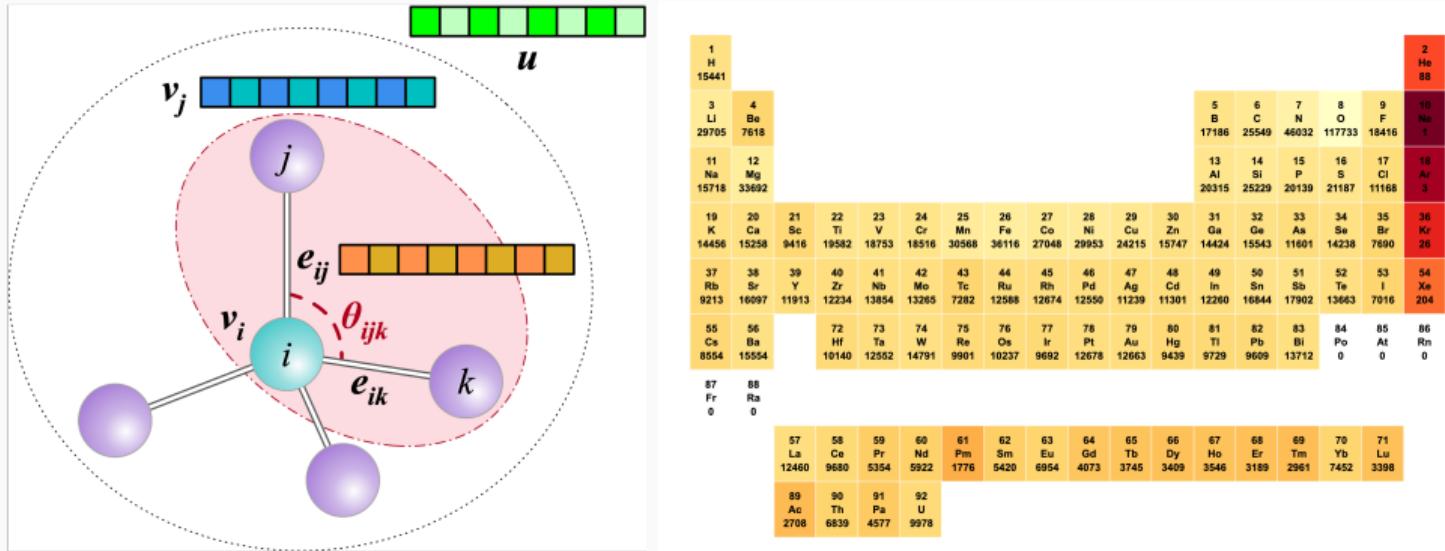


Figure 15: Materials 3-body Graph Network (M3GNet), the first whole periodic table MLIP.[18]

Modeling complex relationships

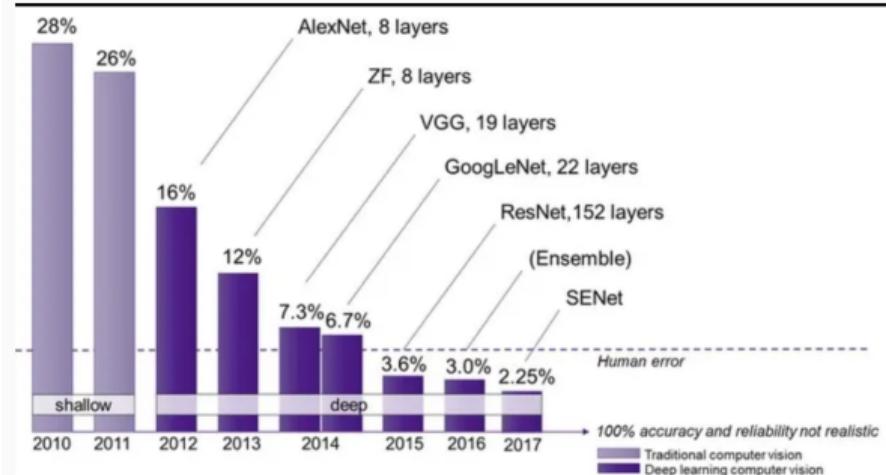
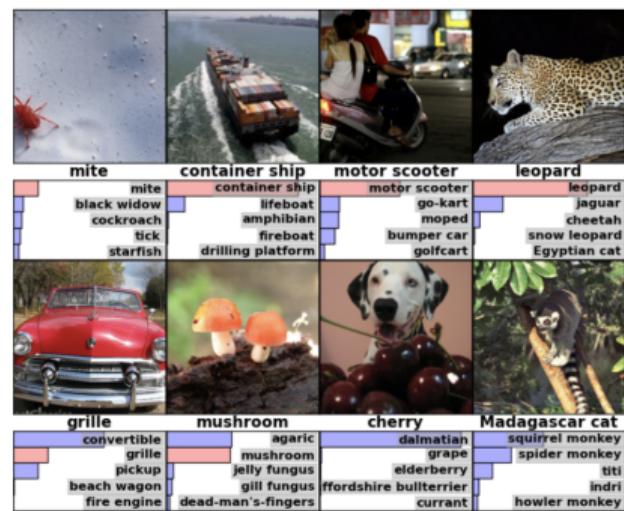


Figure 16: ImageNet (<https://www.image-net.org/>)

Example: Coordination environment from X-ray Absorption Spectra

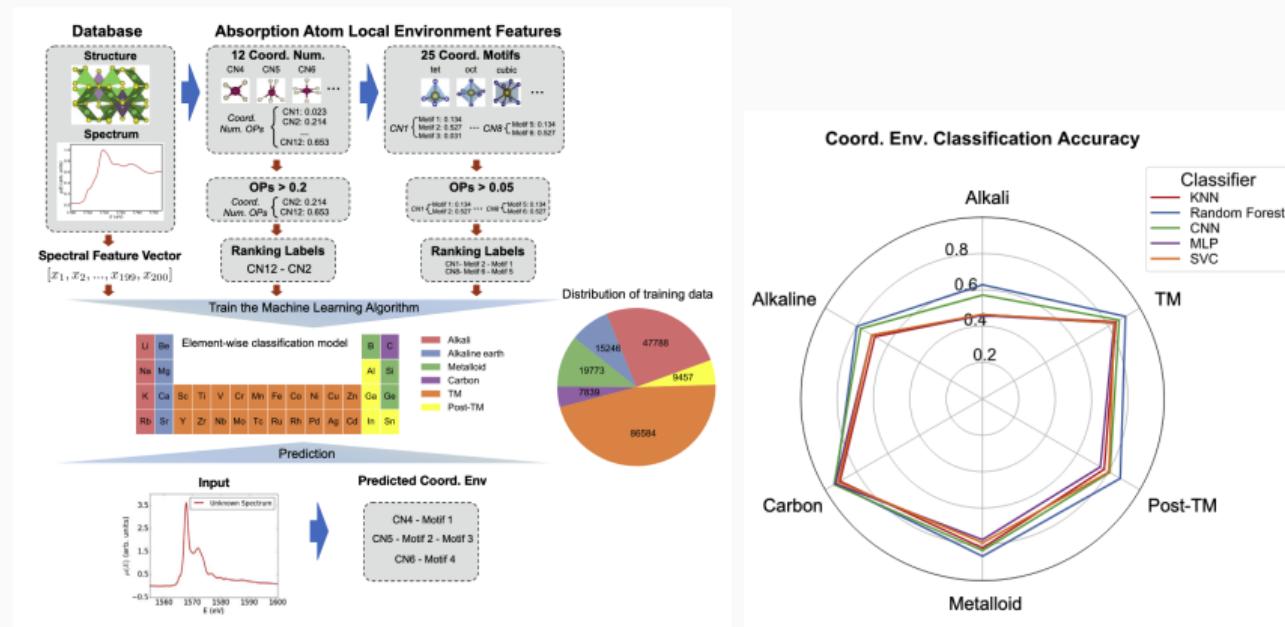


Figure 17: Random Forest Coordination Environment Classification[19]

Other examples

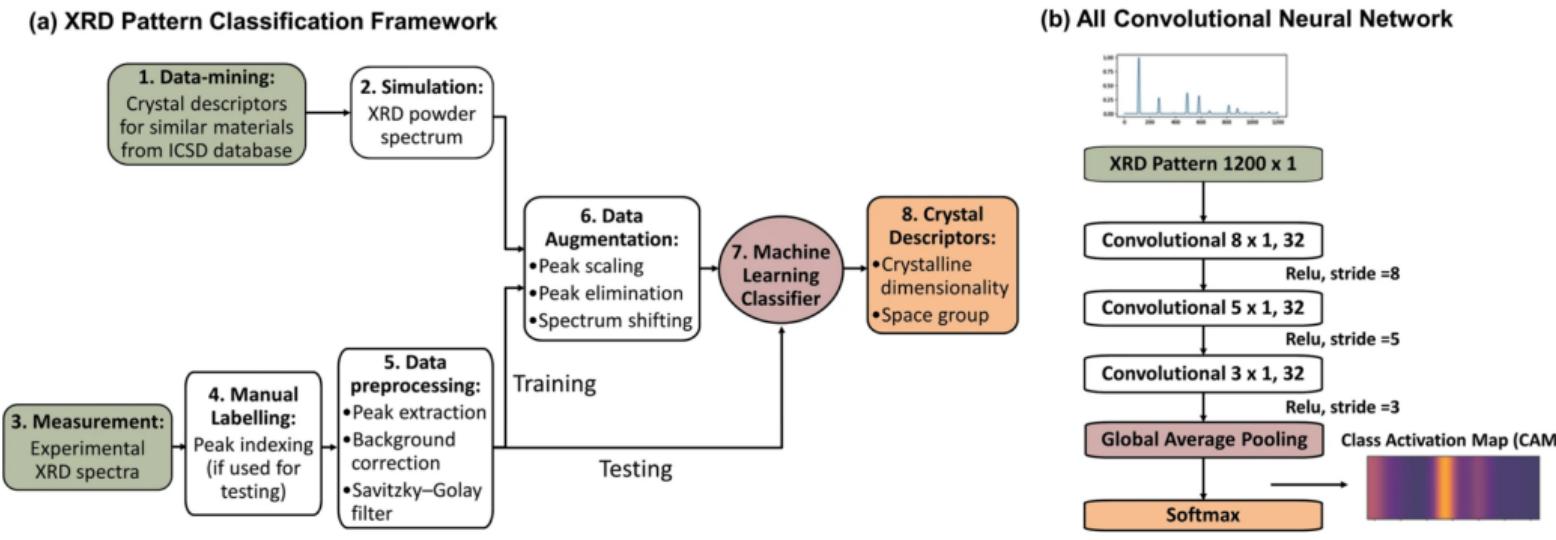


Figure 18: X-ray diffraction data classification with CNNs[20]

Bibliography i

-  Wenhao Sun, Stephen T Dacek, Shyue Ping Ong, Geoffroy Hautier, Anubhav Jain, William D Richards, Anthony C Gamst, Kristin A Persson, and Gerbrand Ceder.
The thermodynamic scale of inorganic crystalline metastability.
Science Advances, 2(11):e1600225–e1600225, November 2016.
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