

Introduction to Data Science in Materials Science

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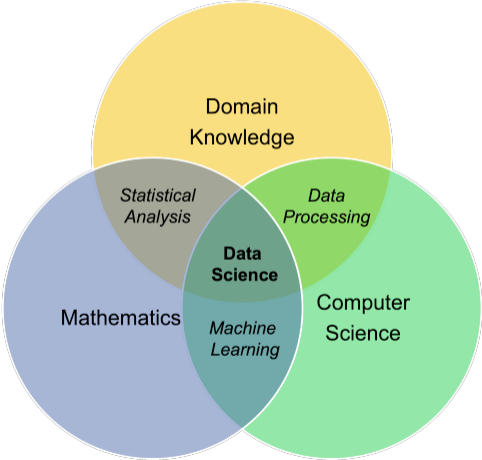
University of California, San Diego

Fall 2023

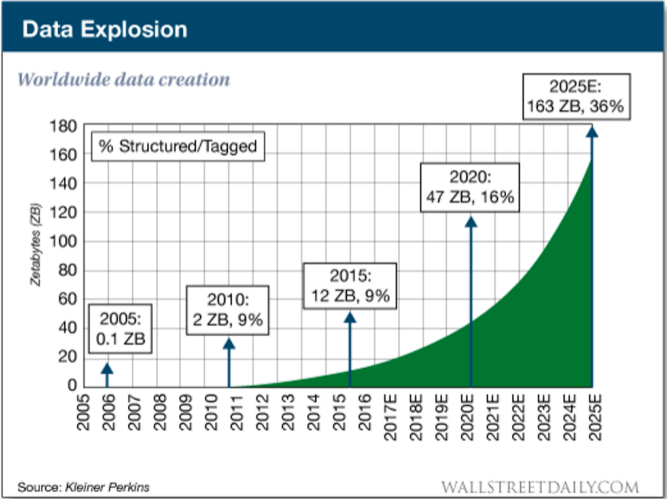
What is Data Science?

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)

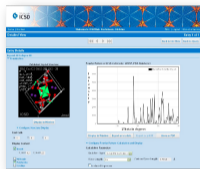


Figure: ICSD: ~200,000 crystals

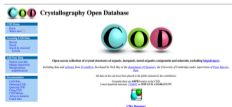


Figure: COD: ~400,000 crystals

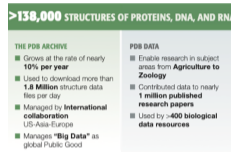


Figure: Protein data bank

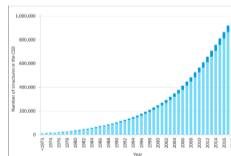


Figure: Cambridge structural database (small-molecule organic crystal structures)

But Quantity and Quality Lags Many Other Fields

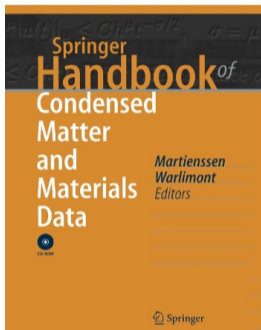


Figure: One of the most comprehensive handbooks on materials data: Density, thermal and electrical conductivity, melting and boiling points, etc., but O(100) binaries and limited ternaries...

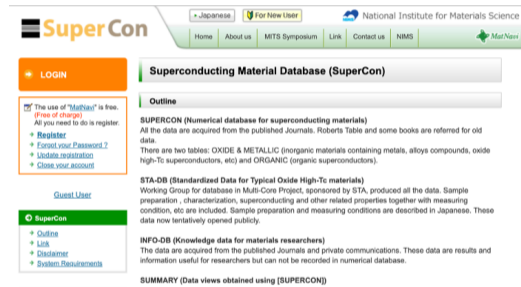


Figure: ~1000+ superconductors (many minor composition modifications). Ref: <https://supercon.nims.go.jp/>

First Principles Materials Computations

Inherently scalable

Generally applicable to any chemistry

Schrodinger Equation

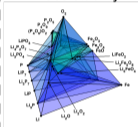
$$E\psi(r) = -\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r)$$

Density functional theory (DFT) approximation

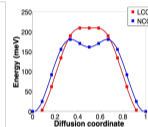


Material Properties

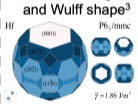
Phase stability¹



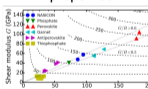
Diffusion barriers²



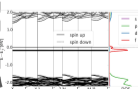
Surface energies and Wulff shape³



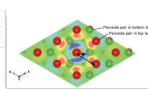
Mechanical properties⁴



Electronic structure⁵

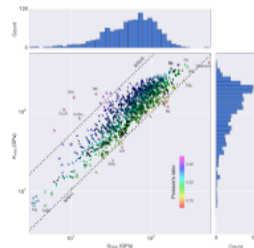
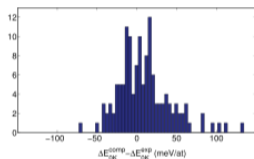
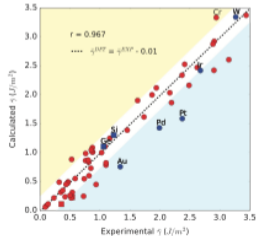
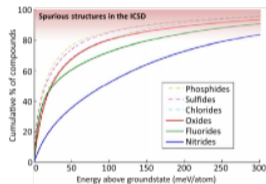


Charge densities⁶



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

	code	Accuracy					
		ELK	WIEN	FP-LMTO	FP-LMTO	FP-LMTO	FP-LMTO
AE	ELK	0.6	0.3	0.3	0.6	1.0	0.9
	wien	0.5	0.3	0.1	0.5	0.9	0.8
	FP-LMTO/1sec2	0.5	0.3	0.1	0.5	0.9	0.8
	FP-LMTO	0.6	0.5	0.5	0.8	0.8	0.4
	FP-LMTO/2+3e	0.8	1.0	0.9	0.8	0.9	0.9
	FP-LMTO/acc	0.5	0.3	0.2	0.4	0.9	0.8
PAW	ORNL/ANENT	0.9	0.8	0.8	0.9	1.3	1.1
	ORNL/ANENT	1.4	1.3	1.3	1.3	1.7	1.5
	ORNL/ANENT	1.6	1.5	1.5	1.5	1.8	1.7
	ORNL/ANENT	0.6	0.6	0.6	0.6	0.9	0.7
	ORNL/ANENT	0.9	0.8	0.8	0.8	1.3	1.1
	ORNL/ANENT	0.6	0.4	0.4	0.4	0.6	0.3
USPP	ORNL/CASTEP	1.1	1.1	1.0	1.0	1.4	1.3
	ORNL/CASTEP	1.1	1.0	1.0	1.0	1.4	1.3
	ORNL/CASTEP	0.7	0.4	0.5	0.5	0.7	0.5
	ORNL/CASTEP	0.5	0.4	0.3	0.3	0.5	0.3
	ORNL/CASTEP	0.3	0.3	0.3	0.3	0.4	0.3
	ORNL/CASTEP	0.3	0.3	0.3	0.3	0.4	0.3
NCPP	ORNL/ANENT	1.5	1.5	1.4	1.4	1.3	1.3
	ORNL/ANENT	2.2	2.2	2.2	2.0	2.3	2.1
	ORNL/ANENT	1.1	1.1	1.1	1.0	1.2	1.1
	ORNL/ANENT	2.0	2.1	2.1	1.9	1.8	2.0
	ORNL/ANENT	0.7	0.7	0.7	0.6	1.0	0.8
	ORNL/ANENT	1.4	1.4	1.3	1.3	1.6	1.5



- (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

OQMD:
The Open Quantum Materials Database

Home Materials Analysis Documentation Download

Newsflash: OQMD v1.1 is out! (Download it [here](#).)

AFLOW
Automatic - FLOW for Materials Discovery

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The Materials Project

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

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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

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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 9, 2011 - 10:09am

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 just about everything humans use -- from buildings and highways to modern necessities. For example, advances in a group of materials called "critical 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 rare "rare earth" elements). With about 50 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

Electronic Structure Click and drag to zoom

Density of States

MATERIAL
TaF₅

Material Details

- Band Magnetic Moment: 0.0000 μ_B
- Formation Energy/Atom: -4.1920 eV
- Energy Above Hull: 0.0000 eV
- Density: 7.18 g/cm³

Explore Materials
Search for materials information by chemistry, composition, or property

Explore Batteries
Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.

Visualize Stability
Generate phase and Pourbaix diagrams to find stable phases and study reaction pathways

Invent Structures
Design new compounds with our structure editor and substitution algorithms

Calculate
Calculate the enthalpy of 10,000+ reactions and compare with experimental values

Database Statistics

133,691 INORGANIC COMPOUNDS	58,329 BANDESTRUCTURES	21,954 MOLECULES	530,243 NANOPOROUS MATERIALS
13,942 ELASTIC TENSORS	3,028 PIEZOELECTRIC TENSORS	3,628 INTERCALATION ELECTRODES	16,128 CONVERSION ELECTRODES

Crystal Structure

Material Properties

- Band Structure
- Volume
- Formation Energy
- Energy Above Hull
- Density
- Stability

Band Structure

Calculated Energy Distribution Functions

Summary

Material	Volume	Formation Energy	Energy Above Hull	Density	Stability
TaF ₅	1.0000	-4.1920	0.0000	7.18	Stable

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.

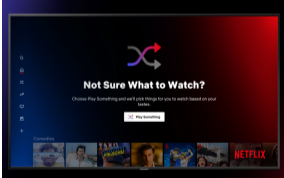
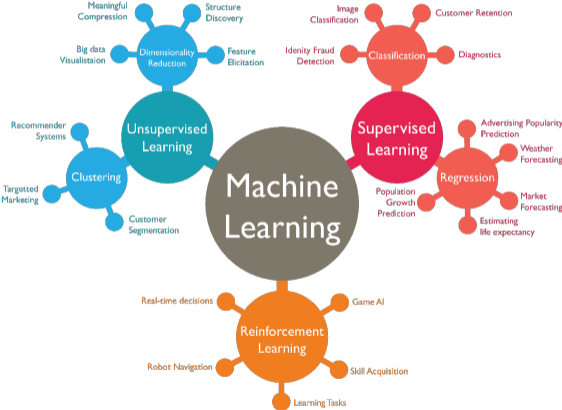
Ranked data

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

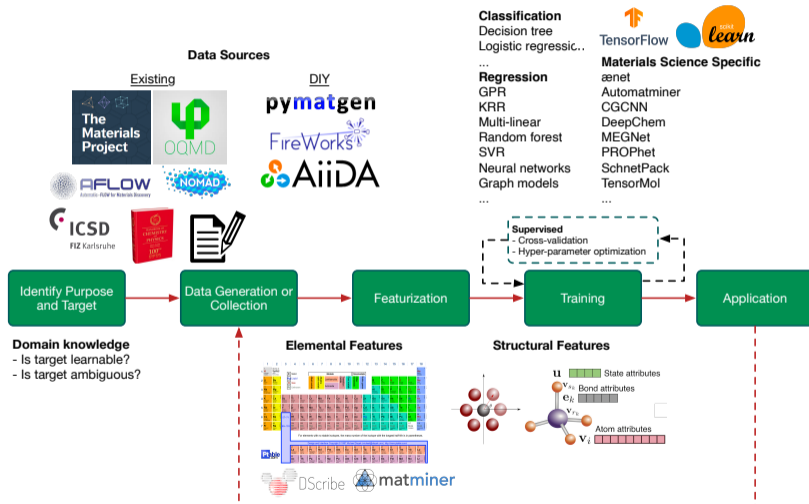
Quantitative Data

- 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?

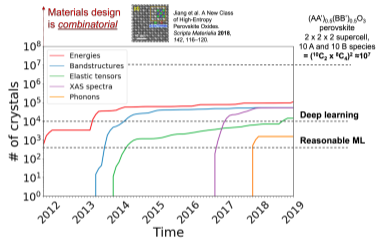


Materials ML Workflow

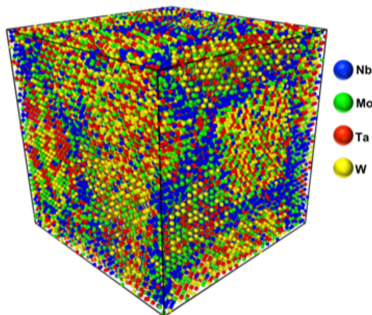


Where is ML valuable in Materials Science?

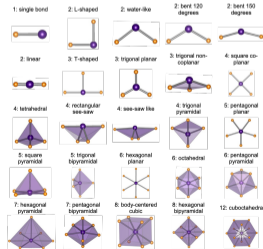
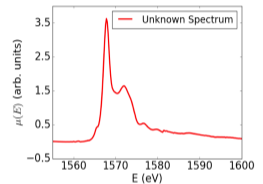
Too many to compute



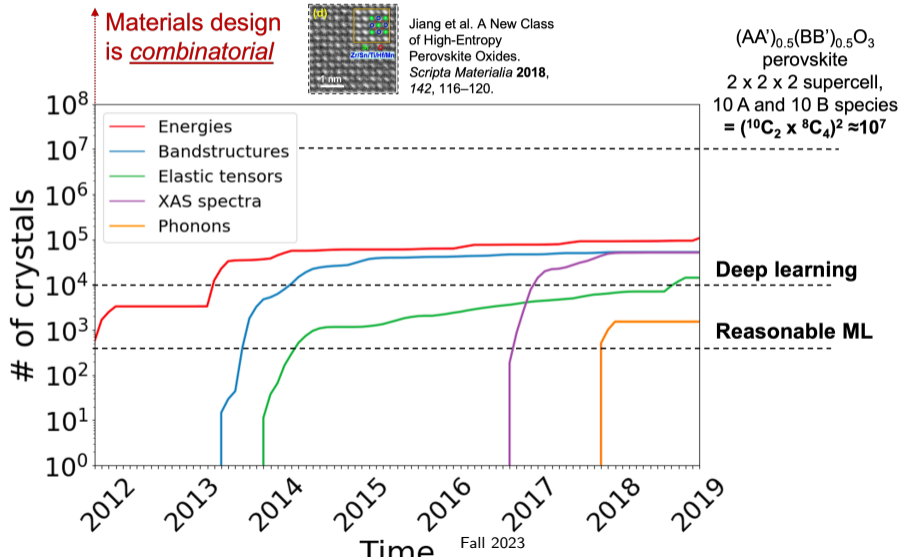
Too big to compute



Too complex to understand.



Data History of the Materials Project



Surrogate models for “instant” property predictions

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

- 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: $0.5 \times 0 + 0.5 \times 4 = 2.0$.
- **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: $0.0 / (3.0 + 2.0 + 3.0 + 0.0) = 0.0$.

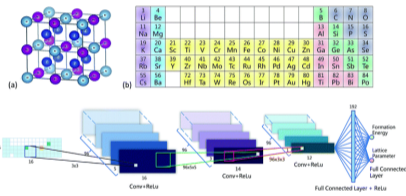
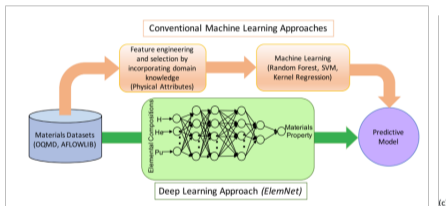


Figure: Jha et al. (2018) Sci. Rep., 8(1), 17593., Zheng, X., et al (2018). Chem. Sci., 9(44), 8426-8432.

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

Structural features

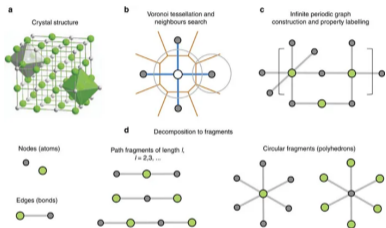


Figure: Property-labelled materials fragments + gradient boosting decision tree.[9]

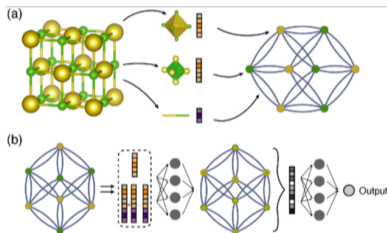


Figure: Crystal graph + graph convolutional neural networks

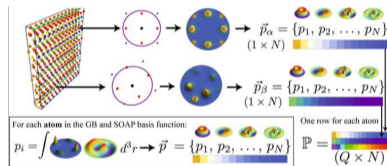


Figure: Smooth overlap of atom positions (SOAP).[10]

Example: Graph-based representations

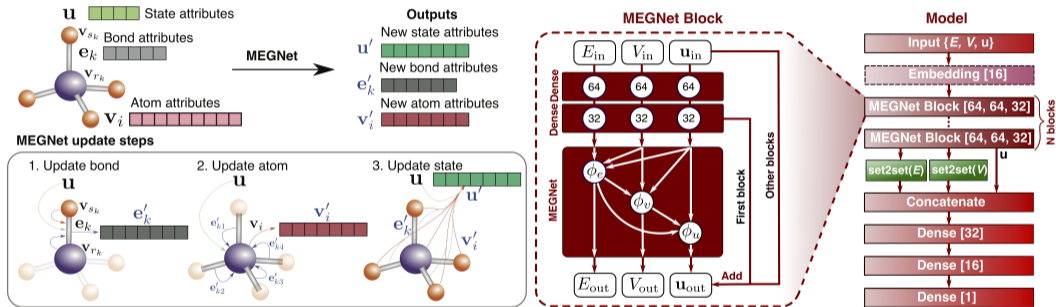


Figure: MatErials Graph Networks (MEGNet).[11]

MEGNet Performance Benchmarks

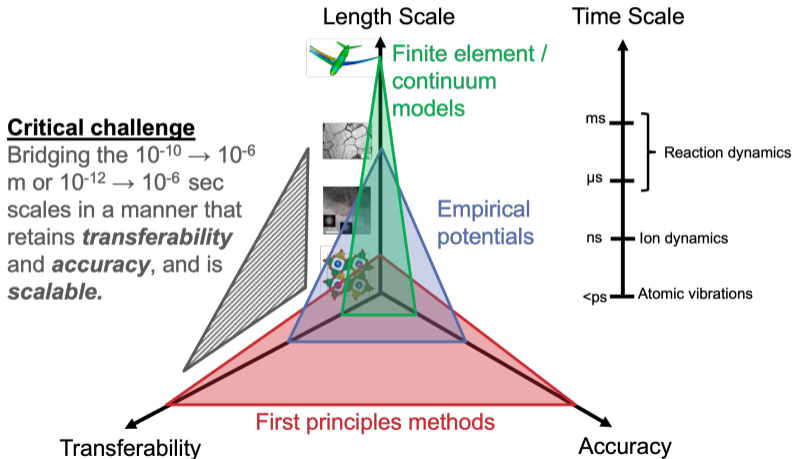
	MEGNET	MEGNET-Simple	SchNet	"Chemical Accuracy"
U0 (meV)	9	12	14	43
G (meV)	10	12	14	43
ϵ_{HOMO} (eV)	0.038	0.043	0.041	0.043
ϵ_{LUMO} (eV)	0.031	0.044	0.034	0.043
C_v (cal/molK)	0.030	0.029	0.033	0.05

Table: 130,462 QM9 molecules

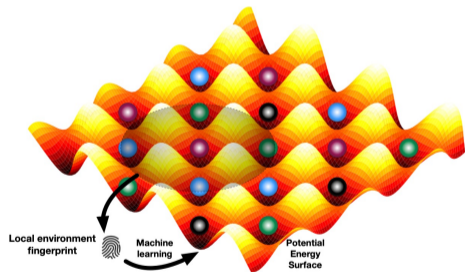
Property	MEGNet	SchNet	CGCNN
Formation energy E_f (meV/atom)	28 (60,000)	35	39 (28,046)
Band gap E_g (eV)	0.330 (36,720)	-	0.388 (16,485)
$\log_{10} K_{VRH}$ (GPa)	0.050 (4,664)	-	0.054 (2,041)
$\log_{10} G_{VRH}$ (GPa)	0.079 (4,664)	-	0.087 (2,041)
Metal classifier	78.9% (55,391)	-	80% (28,046)
Non-metal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

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

Scale Challenge in Materials Science



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

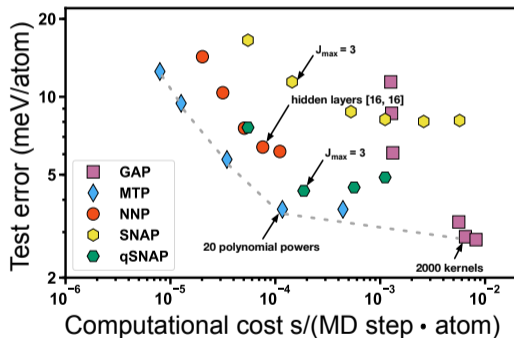
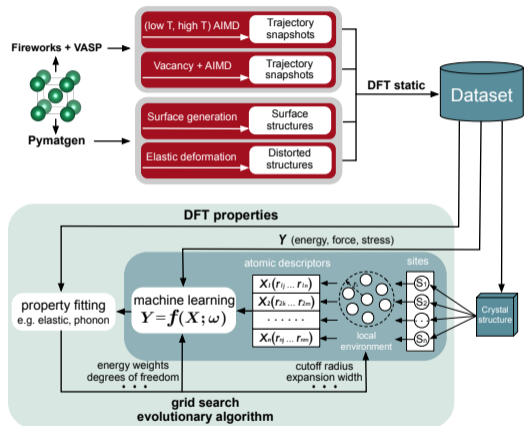


Figure: Automatic workflow for ML-IAP construction and performance benchmarks.[17]

Example: Ni-Mo

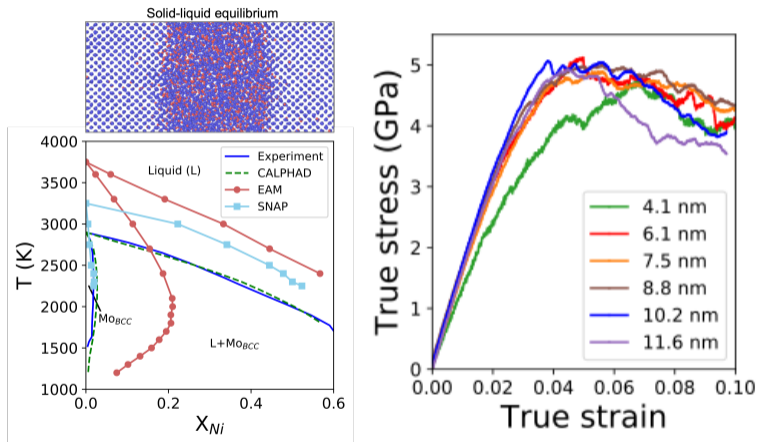


Figure: ML-IAP results on Ni-Mo. (left) Ni-Mo phase diagram. (right) Stress-strain curves as a function of grain size[17]

Modelling complex relationships

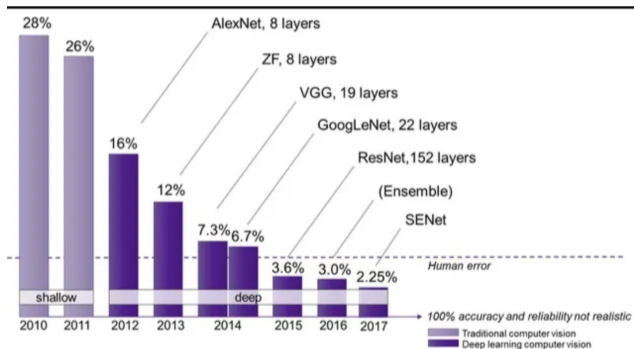
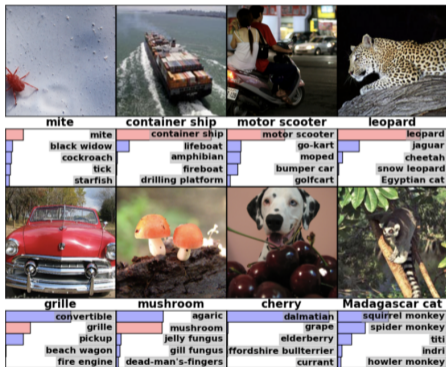


Figure: ImageNet (<https://www.image-net.org/>)

Example: Coordination environment from X-ray Absorption Spectra

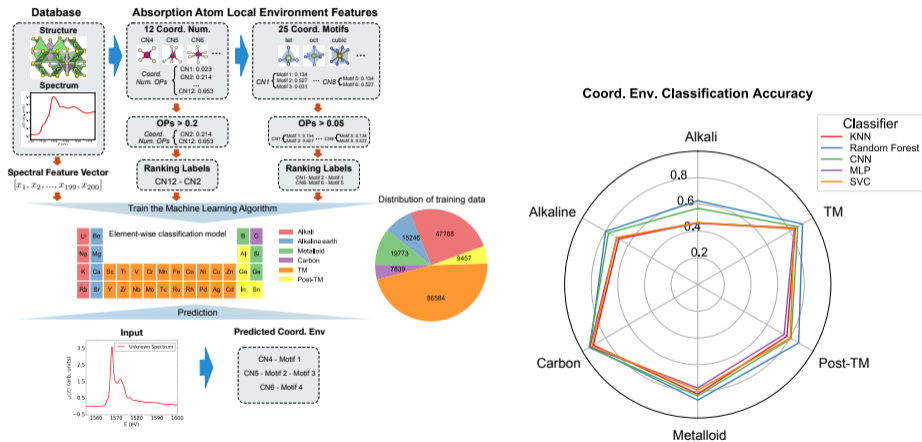
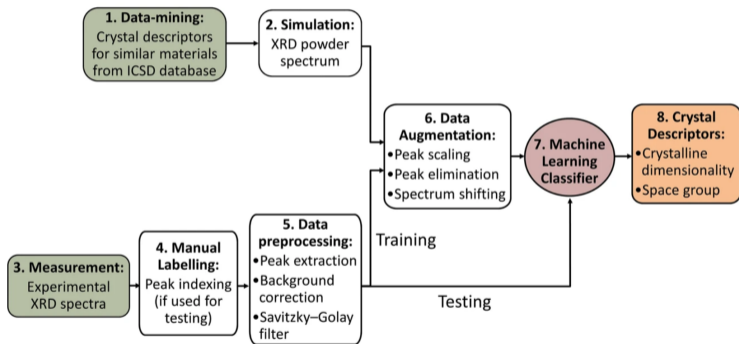


Figure: Random Forest Coordination Environment Classification [18]

Other examples

(a) XRD Pattern Classification Framework



(b) All Convolutional Neural Network

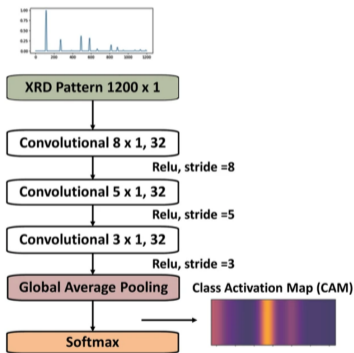





Figure: X-ray diffraction data classification with CNNs[19]

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