Lecture #3: Data in materials science

Slides by Artem Dembitskiy

Previously on

- What is materials informatics
  - Solving materials science problems with **data** science tools
  - HW0 announcement
- Python for materials modeling
  - Automation vs. Manual
  - Intro to ASE and Pymatgen

Goals

- Understand the role of data in materials science
- Provide sources of data
- Introduce the Materials Project database and its API

Agenda

- Experimental data
- Computational data
- Why use someone else's data?
- FAIR principles
- The Materials Project

What is data?

"Data is a representation of information stored in a systematic way for the purpose of inference, argument or decision making"

From An Introduction to Data Analysis by Michael Franke

As materials science researchers, we generate a lot of experimental and computational data

2-3D Images:

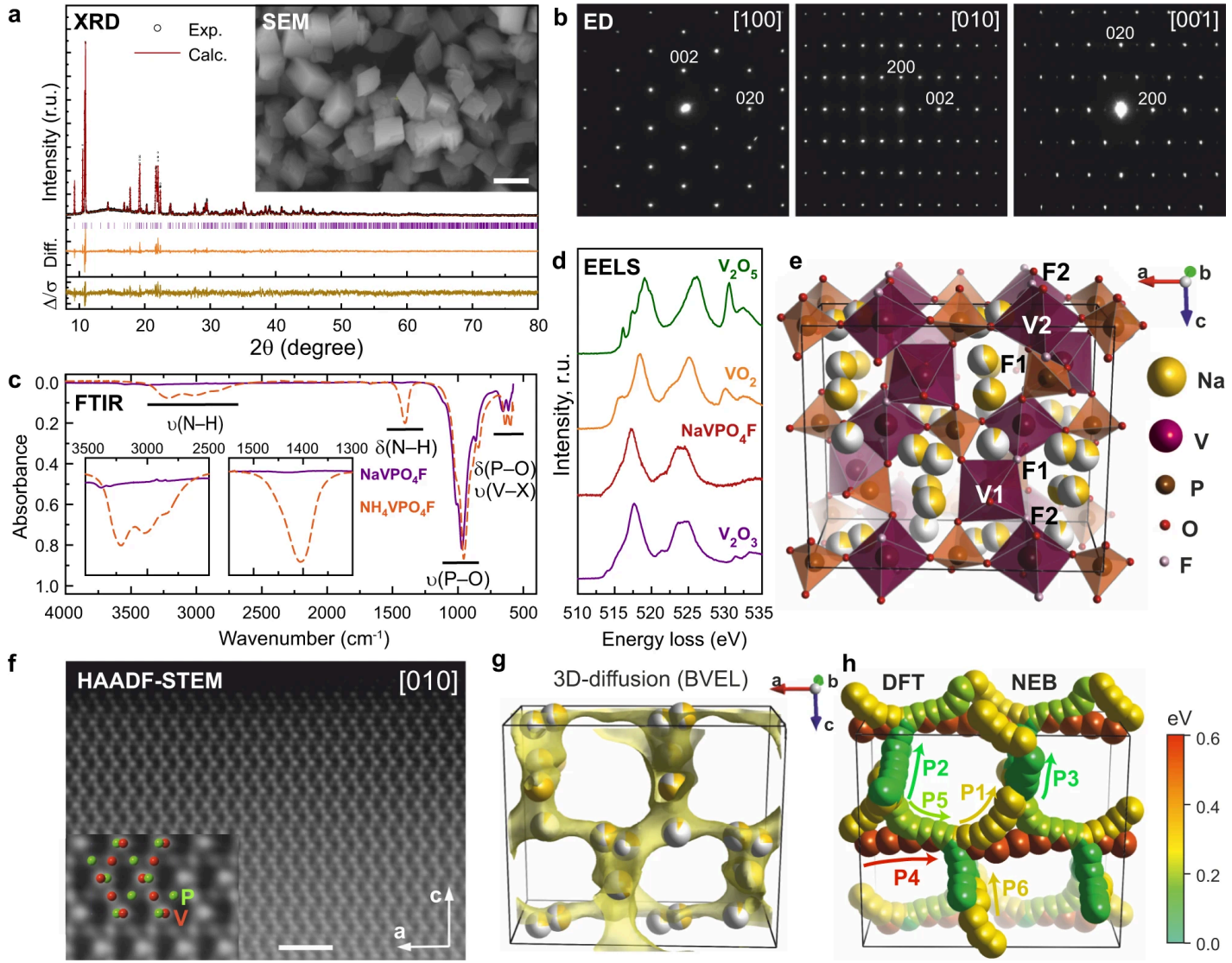
- Electron microscopy images (exp)
- Electron density (exp/comp)

Tabular data

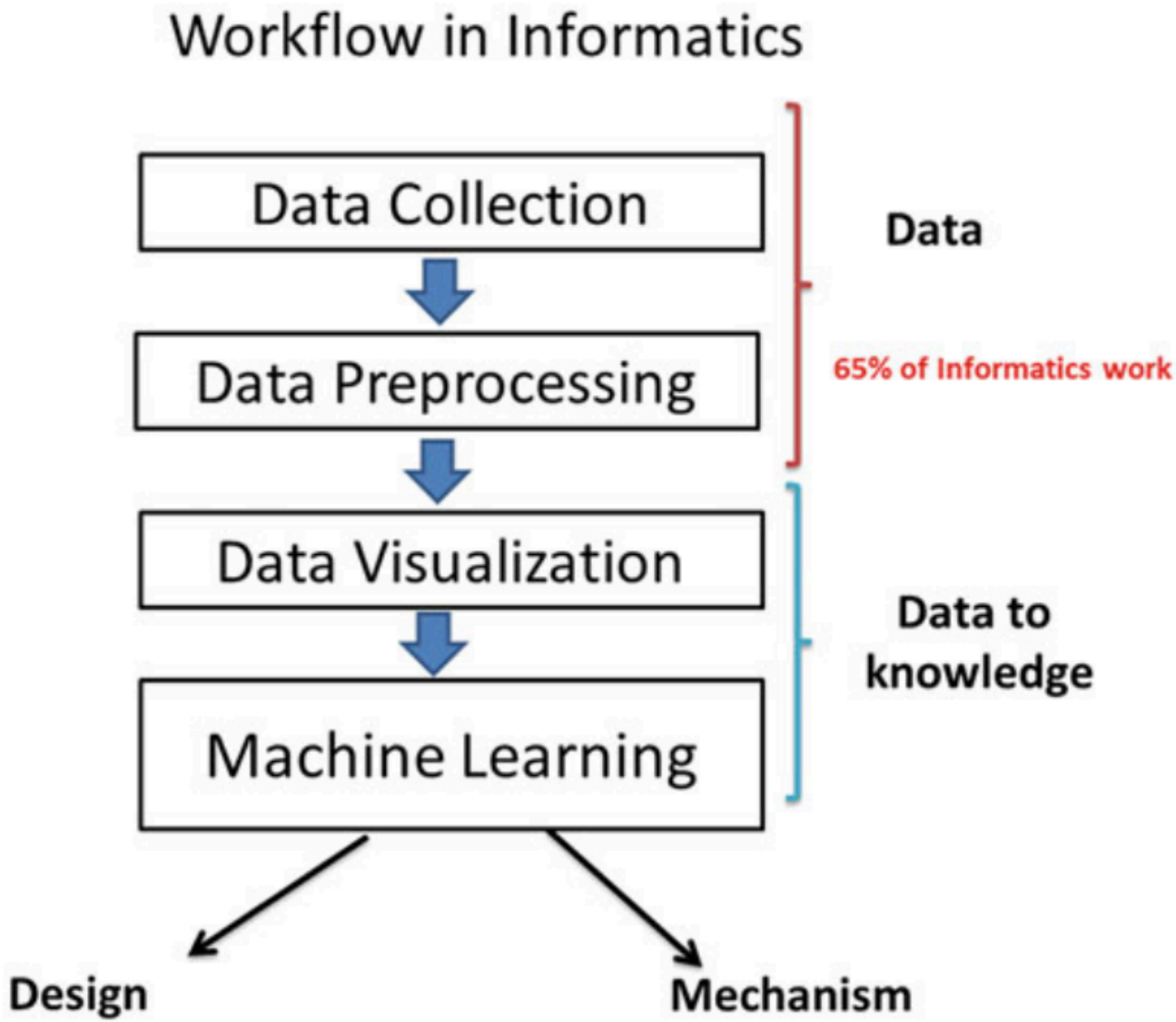
- Eg vs. composition (the last seminar)
- X-ray diffraction pattern (exp/comp)
- Particle size distribution (exp)
- Density of states (comp/exp)
- Energy profile (comp/exp)

Text

- Structure files (exp/comp)



Typical workflow in materials informatics



How to get data?

On your own:

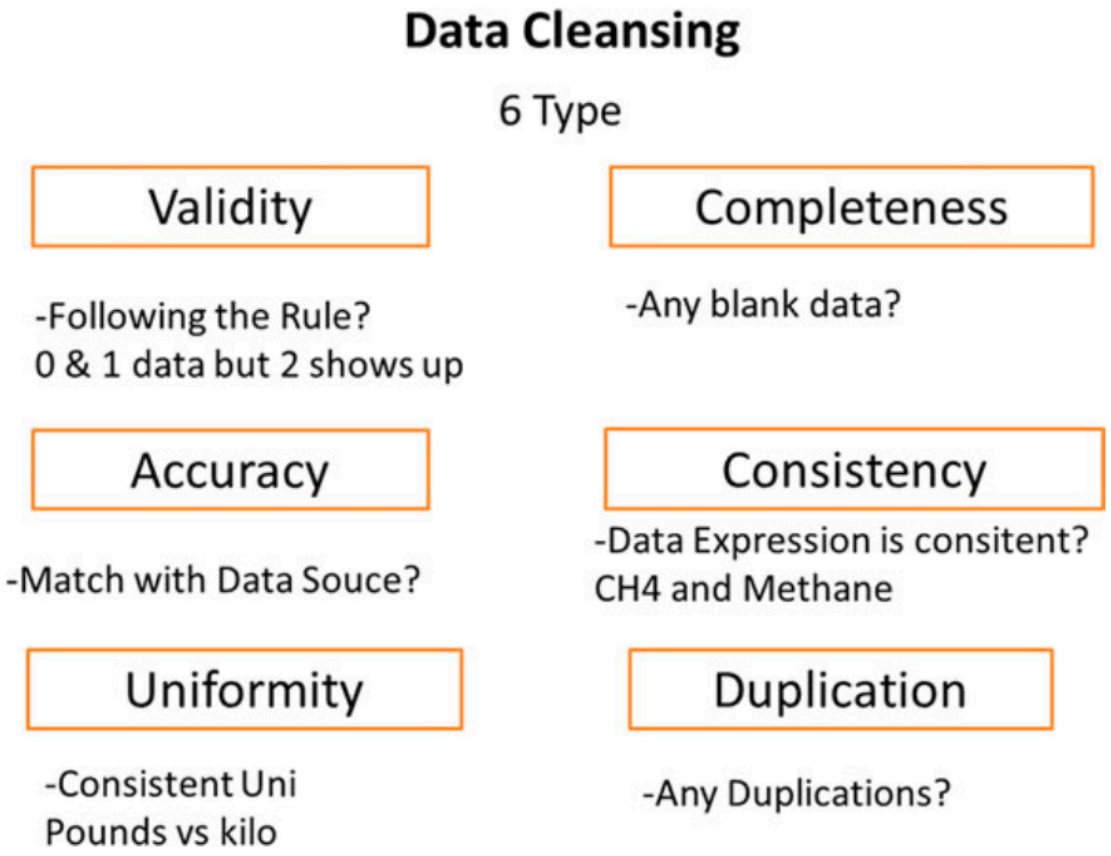
- Manual collection from your experiment or simulation
- High-Throughput experiment or High-Throughput calculations
- Extract from Review Articles: https://github.com/automeris-io/WebPlotDigitizer
- Text Mining using reseach articles: https://www.nltk.org/, chatGPT

From available datasets:

- Data purchase
- Open materials databases

Data preprocessing

- Cleansing
- Augmentation - variations and transformation to extend the dataset.
- Aggregation - integration of multiple datasets



There is a huge amount of materials science data

... scattered across various papers, datasets, databases and websites

Github:

- https://github.com/blaiszik/Materials-Databases

Curated databases

- ICSD: https://icsd.products.fiz-karlsruhe.de/
- COD: https://www.crystallography.net/cod/
- CCDC: https://www.ccdc.cam.ac.uk/
- Materials project: https://next-gen.materialsproject.org/
- The Open Quantum Materials Database: http://oqmd.org/
- AFLOW: http://www.aflowlib.org/
- matbench: https://matbench.materialsproject.org/

...and more

Why use someone else's data?

- guide to your research objective
- reference
- baseline
- insight
- explanation
- enrichment
- time

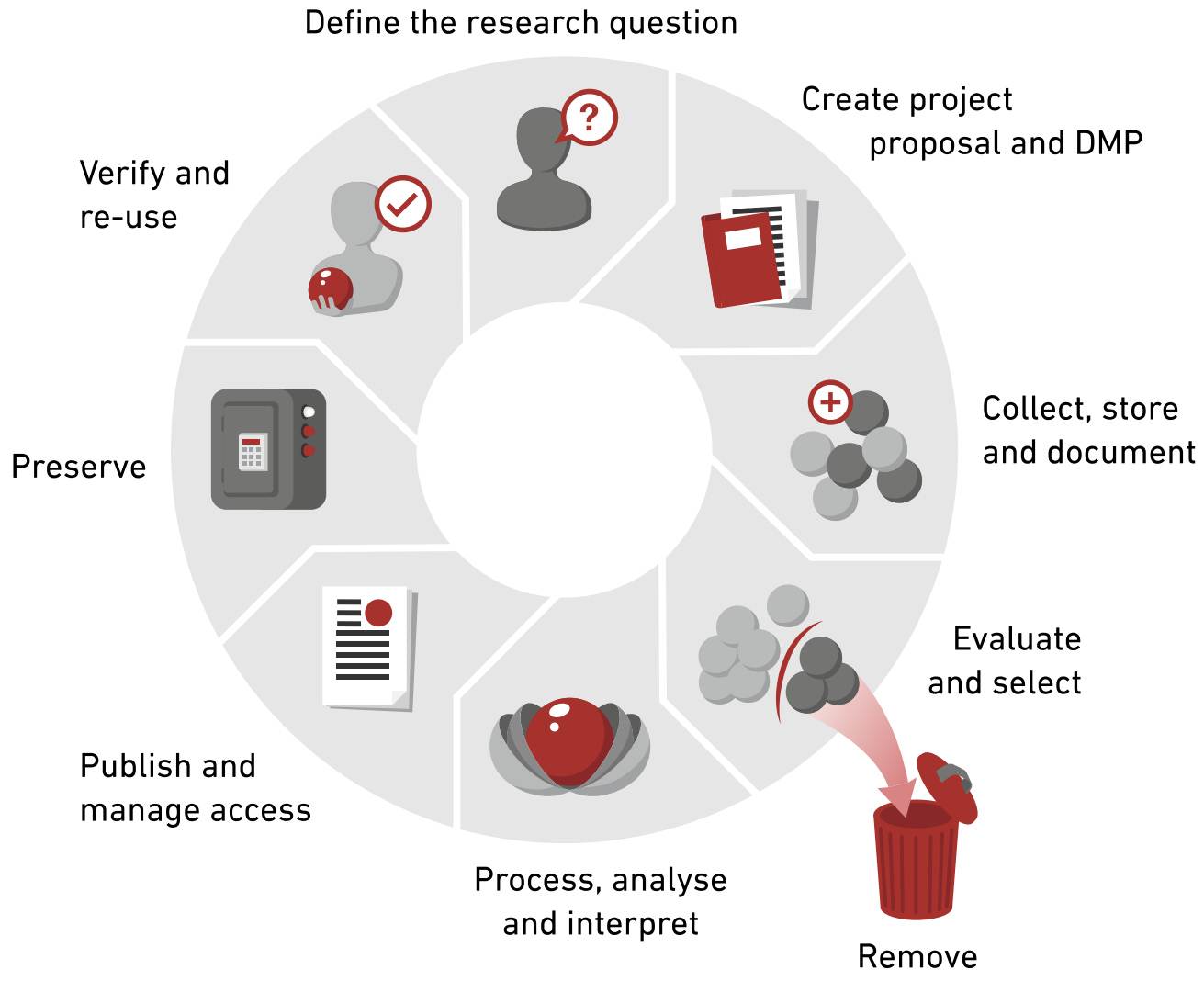


Image source

What do we expect from the data source?

The FAIR Guiding principles

... for scientific data management and stewardship

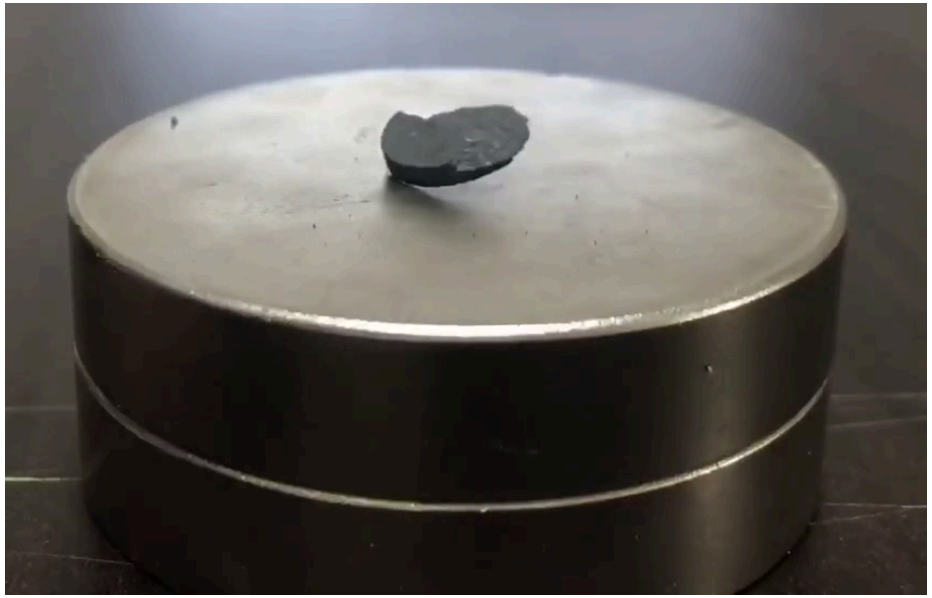
Image source

These principles should guide your projects (and future research)

Bad (toy) example - SuperDuperConductorsDB

- a dataset of superconductivity temperatures of 5,000,000 novel stable crystal structures
- with only transition temperatures and chemical compositions shared
- no crystal structures, no methods provided

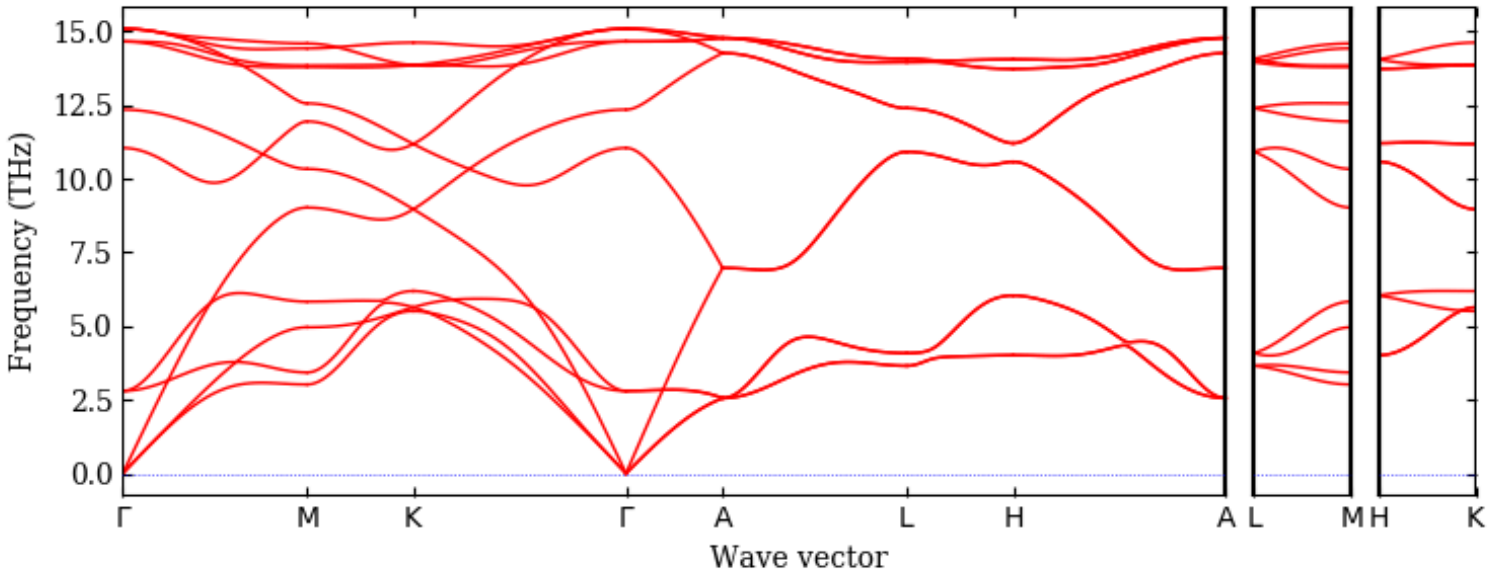
website: https://idontsharemydata.com/



Ok example - phonondb

- phonon dispersion curves calculated for ~10,000 crystal structures
- methods, metadata, structure files provided
- hard to handle the data

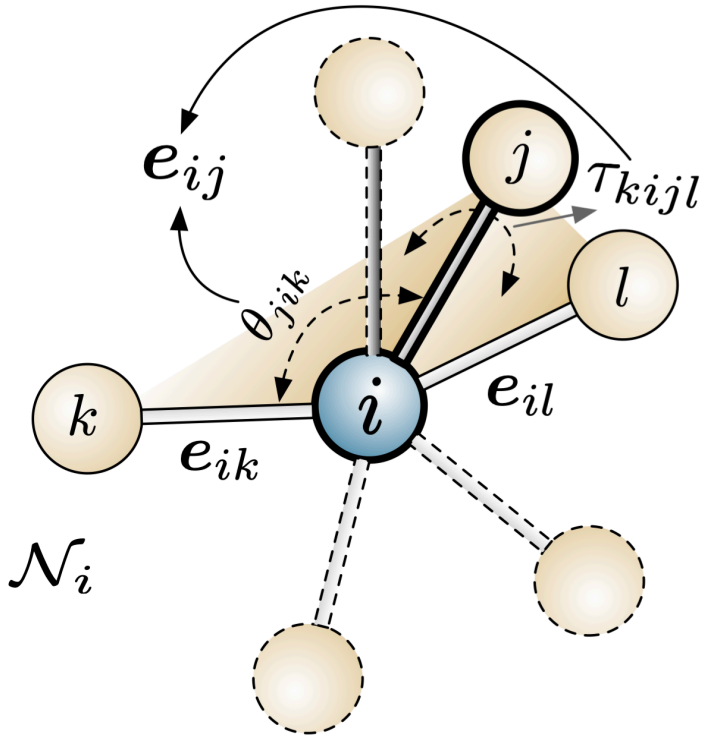
website:
https://github.com/atztogo/phonondb



Good example - matterverse

- ~30,000,000 crystal structures optimized with deep learning potential
- methods, metadata, structure files provided
- has the platform
- REST API is not that good

website: https://matterverse.ai/about

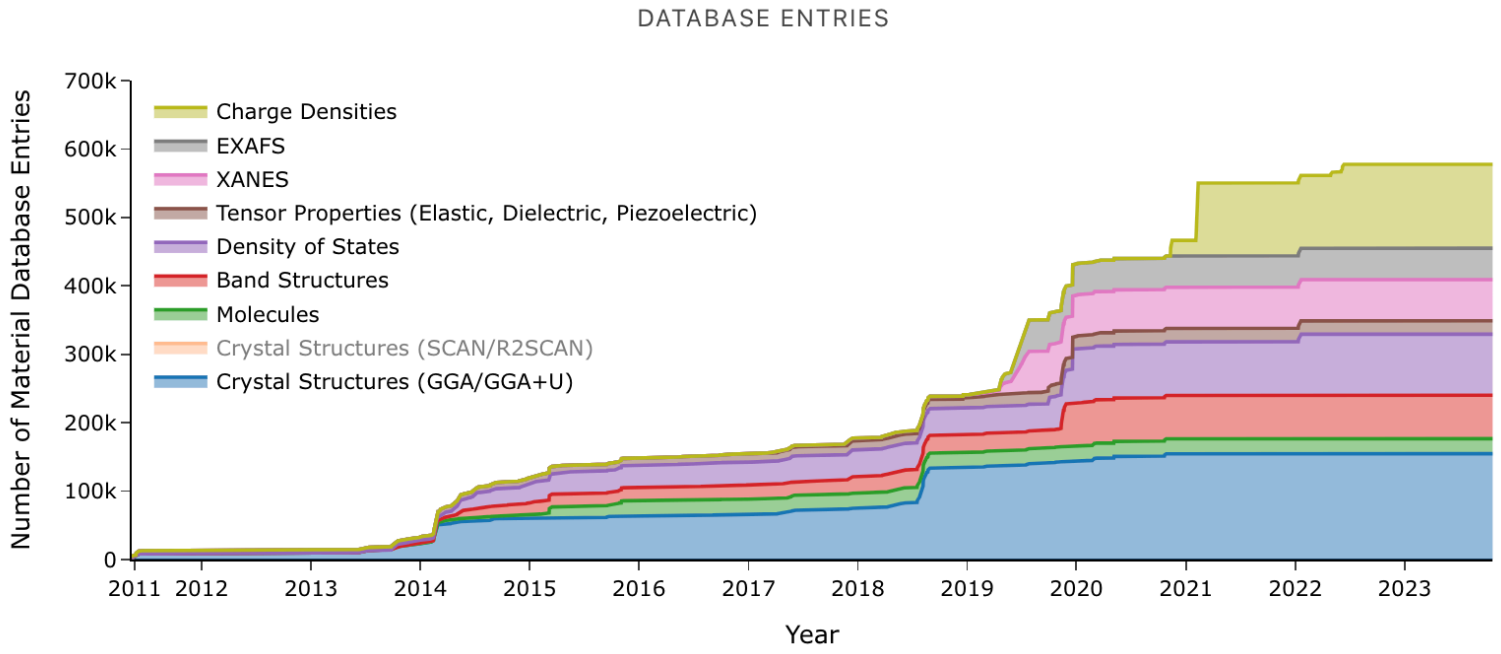


Brilliant example - The Materials Project (MP) database

- ~150,000 crystal structures
- high quality density functional theory calculations
- "provides one of the largest publicly available data set of computed materials properties"
- methods, metadata, structure files provided
- handy platform
- good REST API

We will learn how to use it during today's seminar

website: https://next-gen.materialsproject.org/



What can we do with this data?

- Structure files
  - Input for your calculations
- Calculations results
  - Correlation analysis
  - Comparison
  - Extract more data
  - Fit a surrogate model (seminar #5)
  - Screening
  - Thermodynamics
    - Formation energies
    - Phase diagrams
    - Stability

Review of computational approaches to predict the thermodynamic stability of inorganic solids

The MP data access - simple

- you need your API key
- and python

Each material in the database has an identifier (mp_id).

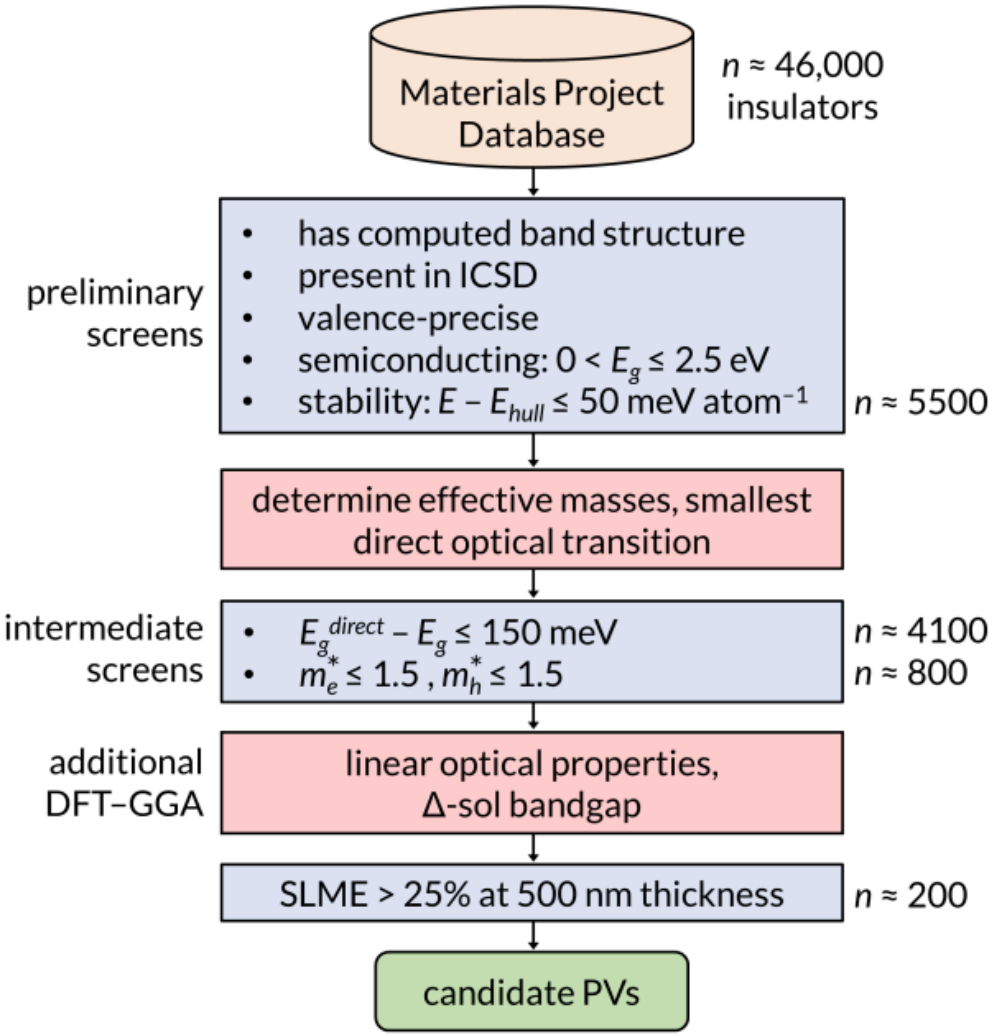
```
from mp_api.client import MPRester

with MPRester(api_key="your_api_key_here") as mpr:
    # retrieve SummaryDocs for a list of materials
    docs = mpr.summary.search(material_ids=["mp-149", "mp-13"])
```

The MP's data usage example

Screening inorganic PVs

- Screened database
- Identified candidates
- Calculated properties of interest for ~800 compounds
- Shared the data



Candidate Inorganic Photovoltaic Materials from Electronic Structure-Based Optical Absorption and Charge Transport Proxies

A few words about Density Functional Theory (DFT) before the MP database seminar

- Quantum-Mechanical approach to calculate the electronic structure (ground state electron density) of materials
- The most popular method in materials modelling
- The main (most important) data generator in computational materials science
- Has high predictive power, but:
  - scales as O(N^3), N - number of electrons in a system
  - requires a lot of compute
- Out of the scope of this course
- Consider Computational Chemistry and Materials Modeling course (MA060008) for learning fundamentals of DFT

Take home message

- There are many (open) sources of materials science related data
- Using someone else's data can help guide or improve your research
- Consider the FAIR principles for sharing your own data

Resources

https://github.com/sedaoturak/data-resources-for-materials-science?tab=readme-ov-file

https://github.com/sp8rks/MaterialsInformatics/blob/main/course_notes/5. Materials Data Repositories.pdf

https://matbench.materialsproject.org/