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:

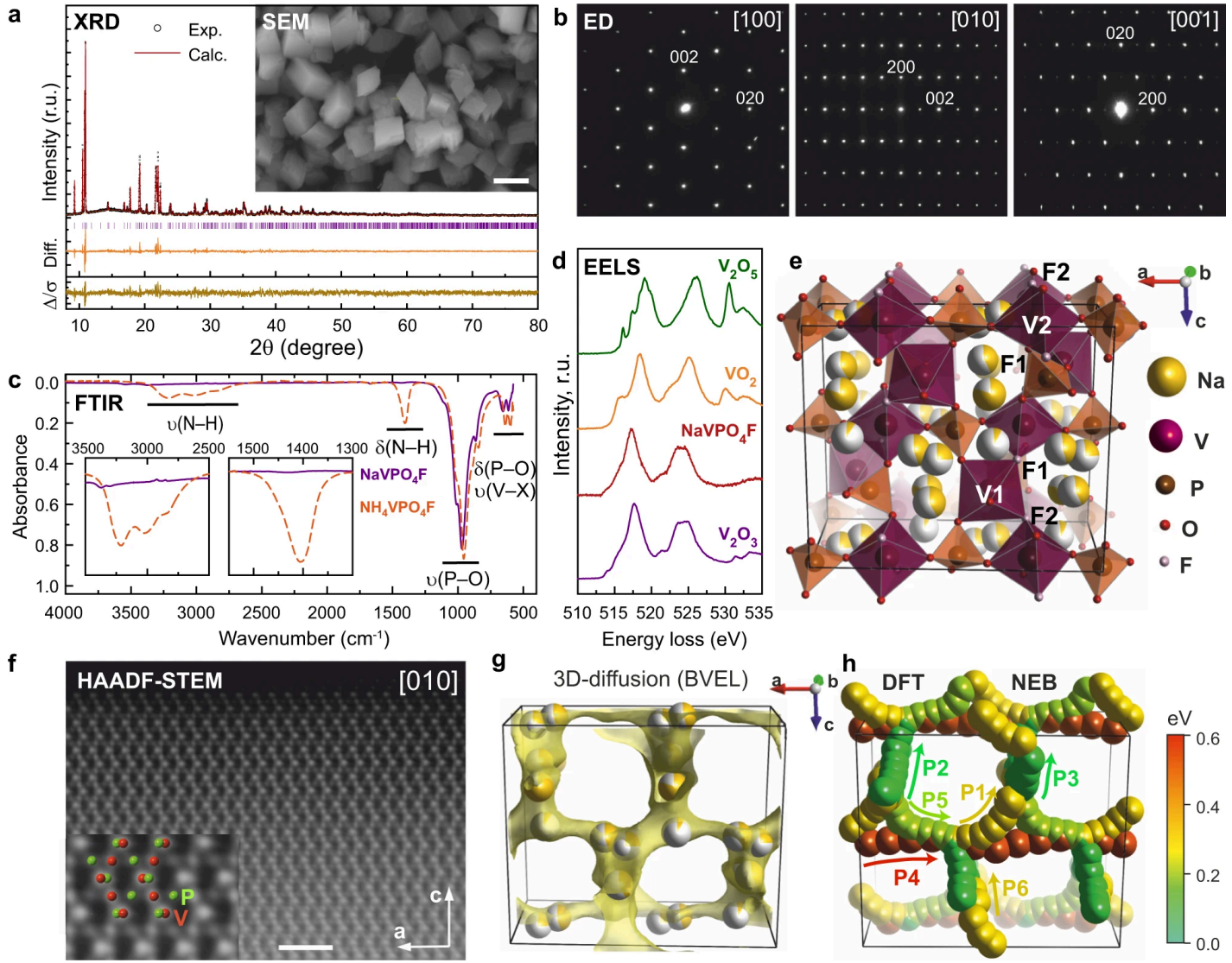
- Electron microscopy images (exp)
- Electron density (exp/comp)

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)



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

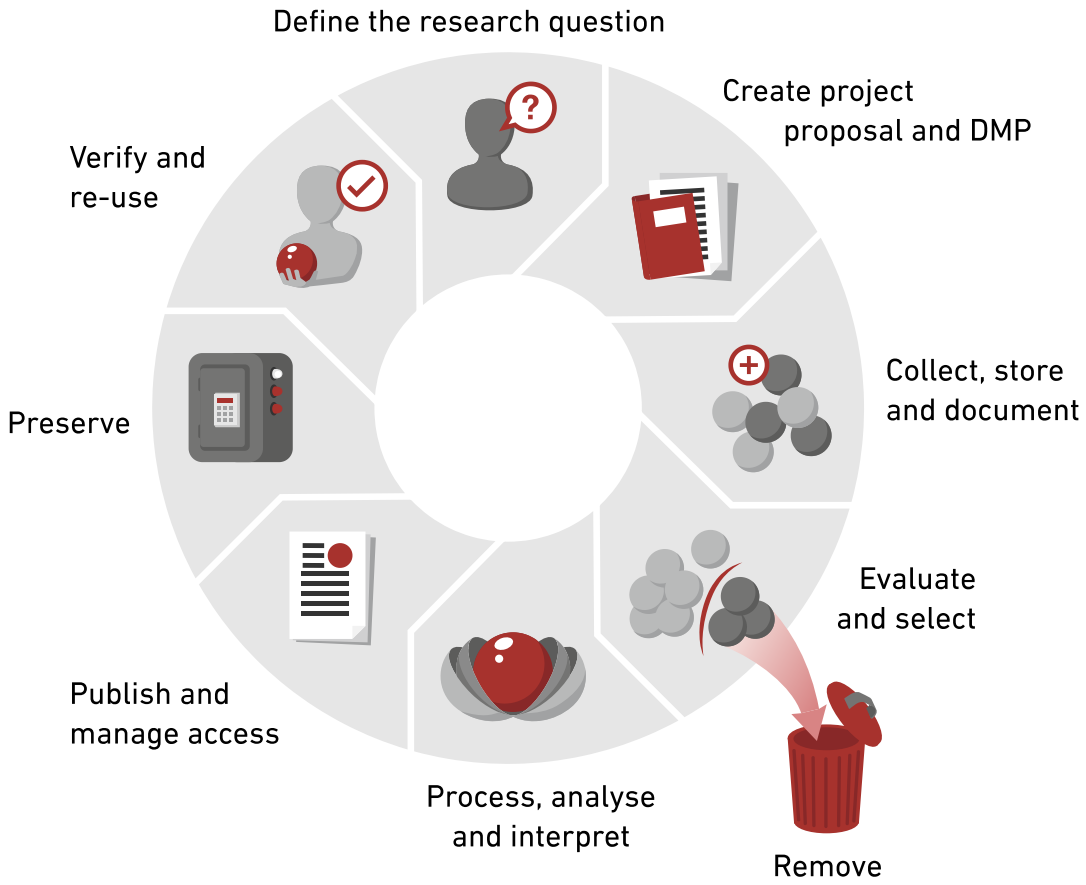


Image source

What do we expect from the data source?

The FAIR Guiding principles

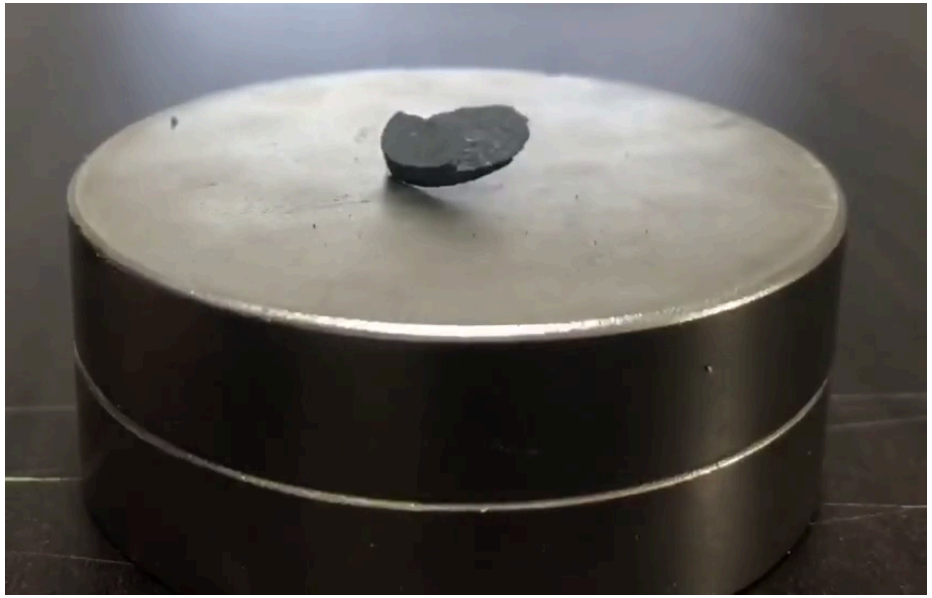
... for scientific data management and stewardship

Image source

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/

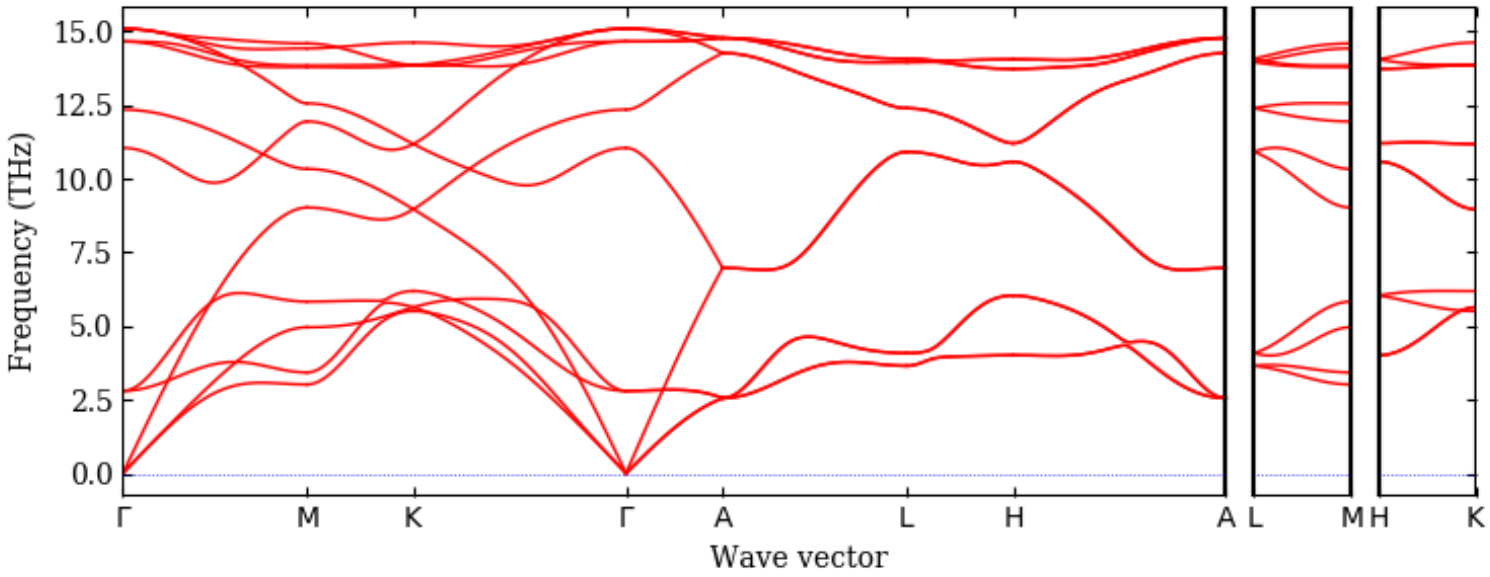


These principles should guide your projects (and future research)

Ok example - phonondb

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

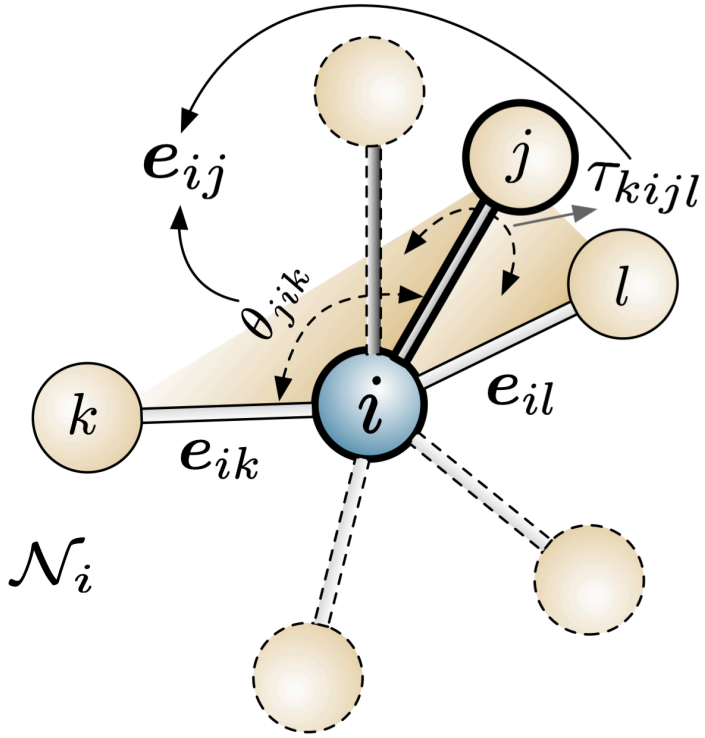
website:
https://github.com/atztogo/phonondb



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

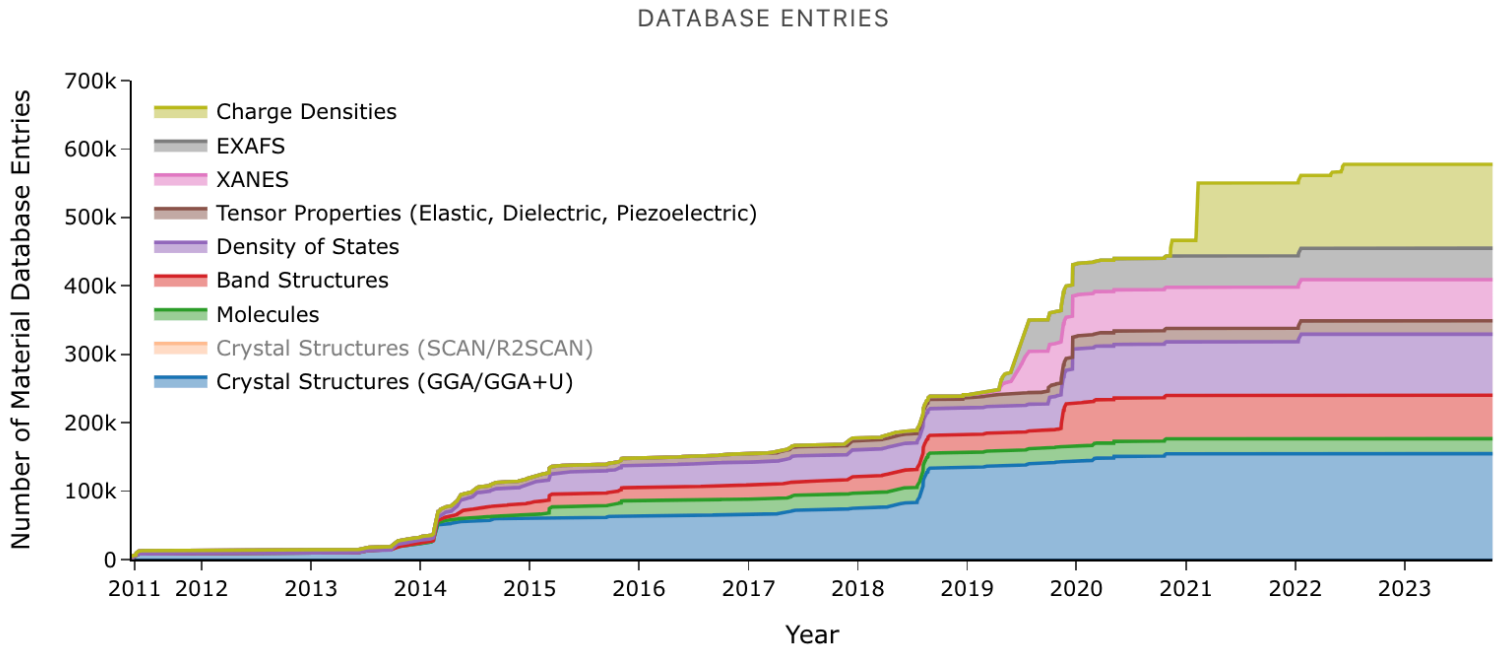


Brilliant example - The Materials Project (MP) database

- ~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/



The MP data access - simple

- you need your API key
- and python

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

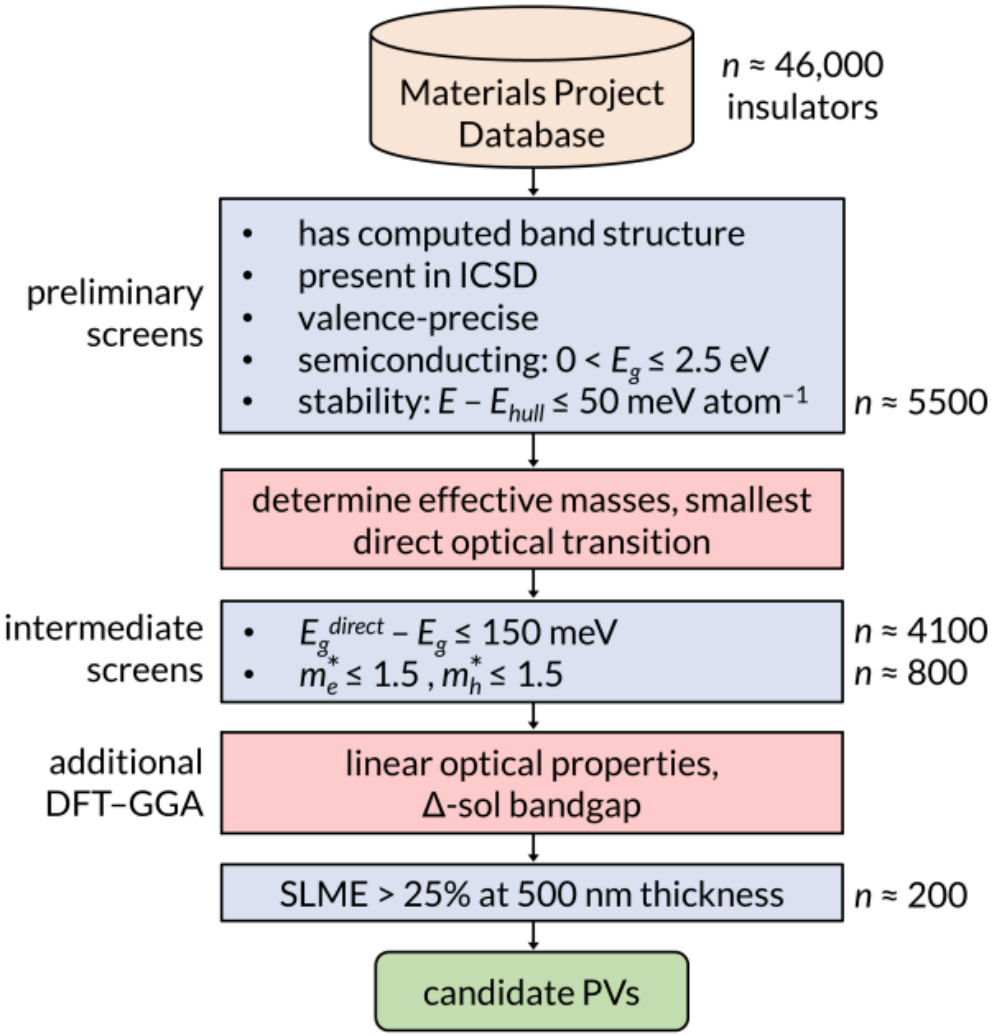
```
from mp_api.client import MPRester

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
- 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 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/