# Lecture #2: Python for atomistic materials modeling

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# Previously on

- What is materials informatics
- Python crash course
- HW0 announcement

# Goals

- Introduce python libraries for materials modeling
- Explain the advantages of using programming over the manual approach

# Agenda

- Materials modeling toy example
- Why use python?
- ASE and Pymatgen

## Toy example: Band gap vs. X in cubic LiX, X = F, Cl, Br, I

Task

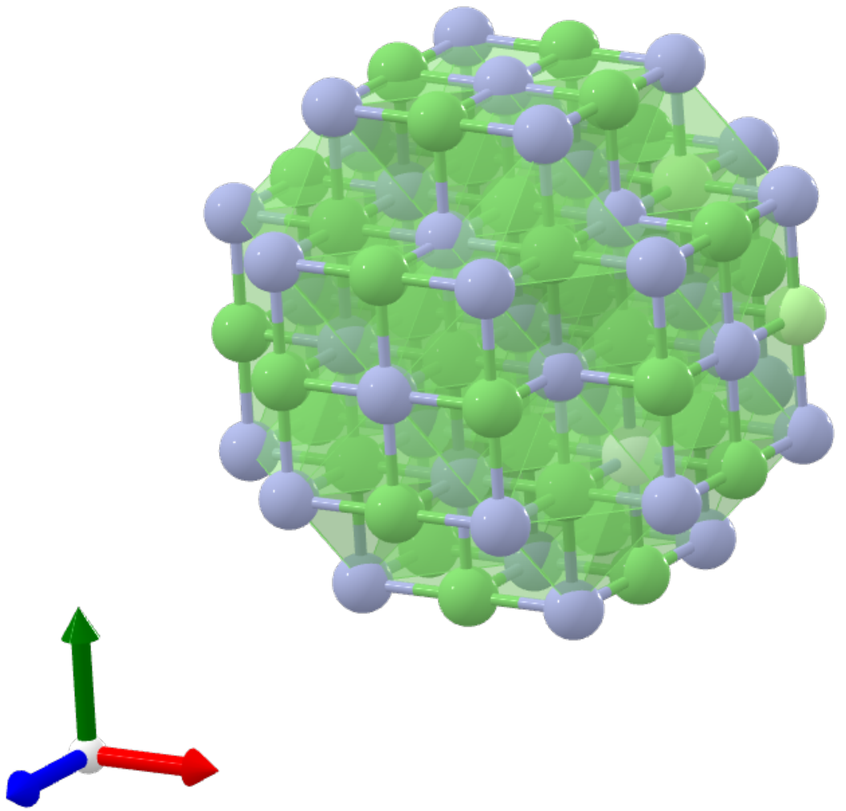
- Calculate a band gap of LiX using a software “Y"
- Perform correlation analysis
- Explain the trend

The software "Y" takes the following input files:

- structure file
- parameters of the calculation
- other specific files

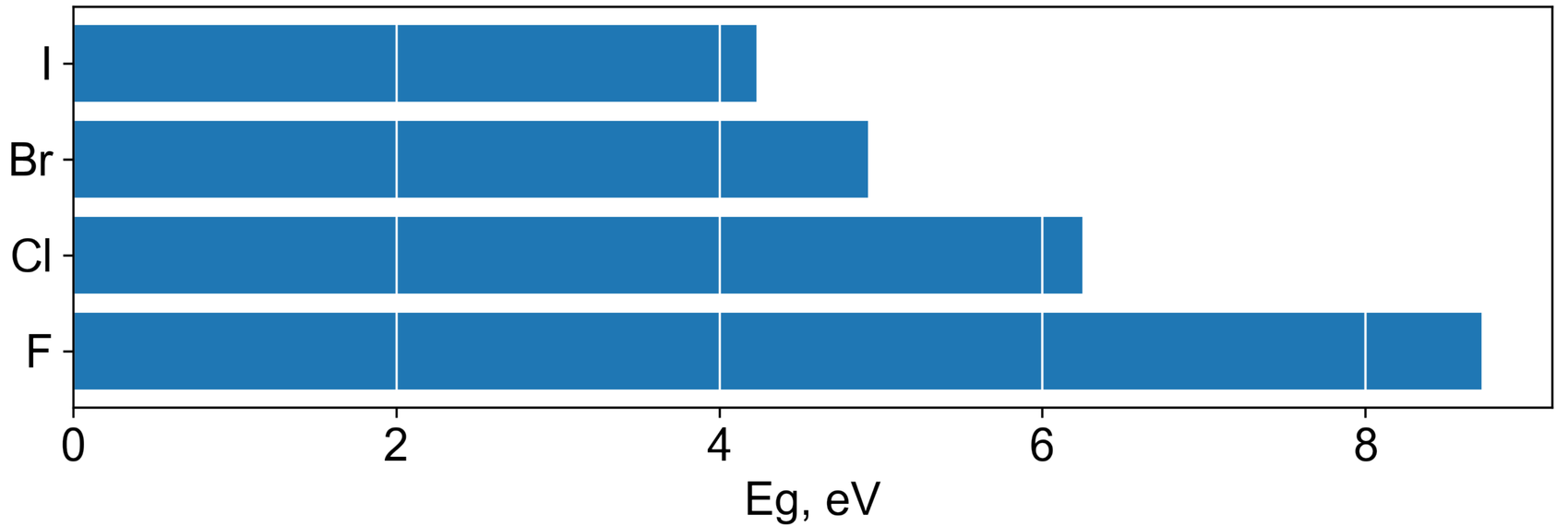
... and outputs:

- 100,000 lines of text
- and one of these contains the $E_g$ value



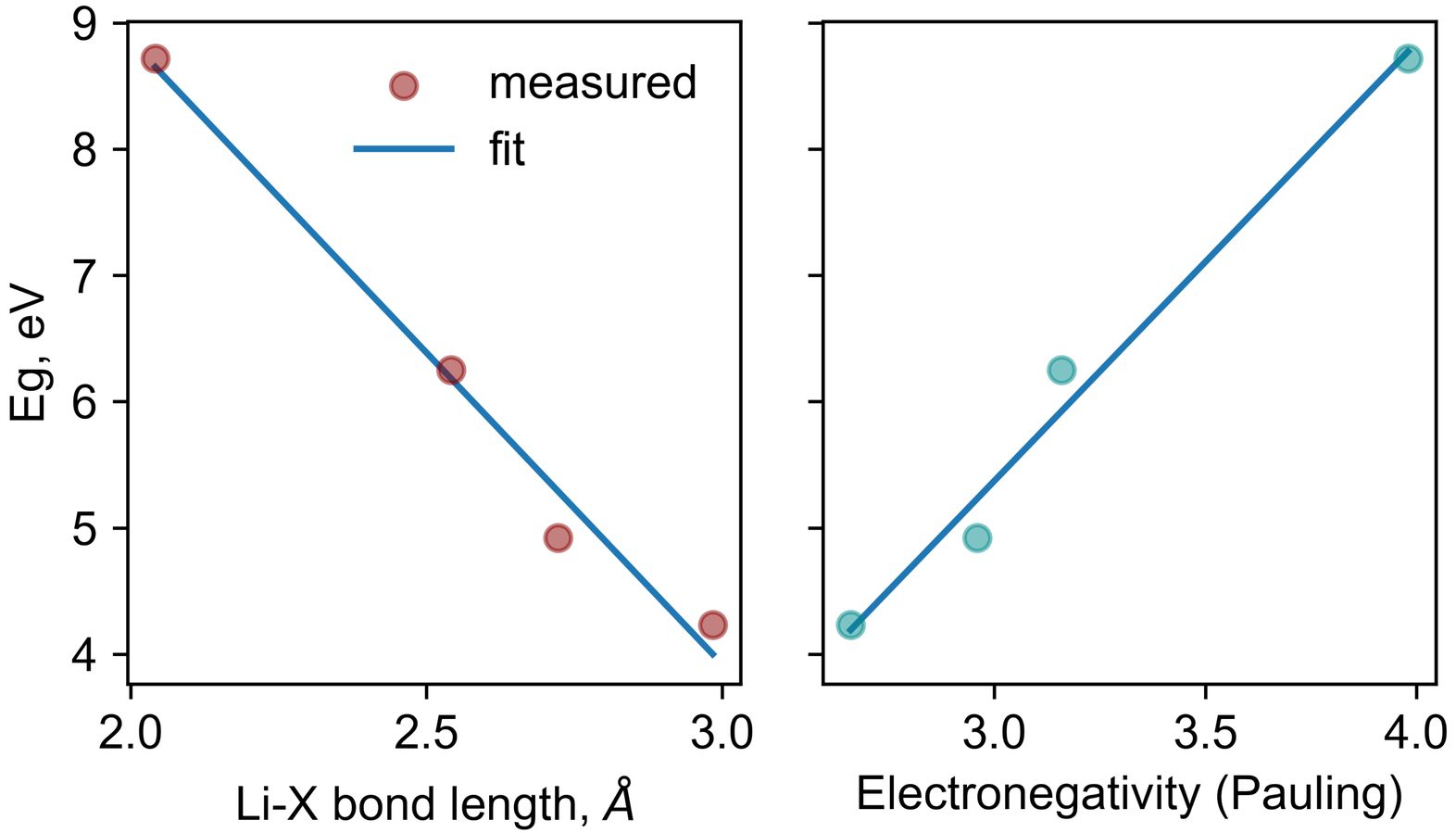
**The trend**

The higher atomic number the lower $E_g$



## Correlation analysis

- Li-X bond length vs. Eg
- Electronegativity (X) vs. Eg



## Workflow

- Get(Create) structure file
- Prepare input files
- Run calculations
- Parse output
- Repeat the above steps for other structures
- Collect observables
- Analyze correlations
- Make conclusions

# Which step takes the longest?

# Which can be automated?

# Manual vs. Automation

## Manual

- Typing input files by hands
- Getting output data by opening files in text editors and copy/paste numbers
- Analysis of output data using Excel and Origin-like programs
- Relying on programs with graphical interface (in some cases its is efficient but in many cases you need to press many buttons every time to accomplish routine tasks )

**Slow, easy to make a mistake, boring for repeating tasks**

When there's a task that can be done manually in 10 minutes but you find a way to automate it in 10 days

# Manual vs. Automation

## Automation

- All input files are created by scripts (only small changes are needed)
- Comprehensive and very flexible analysis specific for your needs
- Easy reuse of code for routine tasks
- Information can be stored in a database
- Takes more time in the beginning, but then is much faster

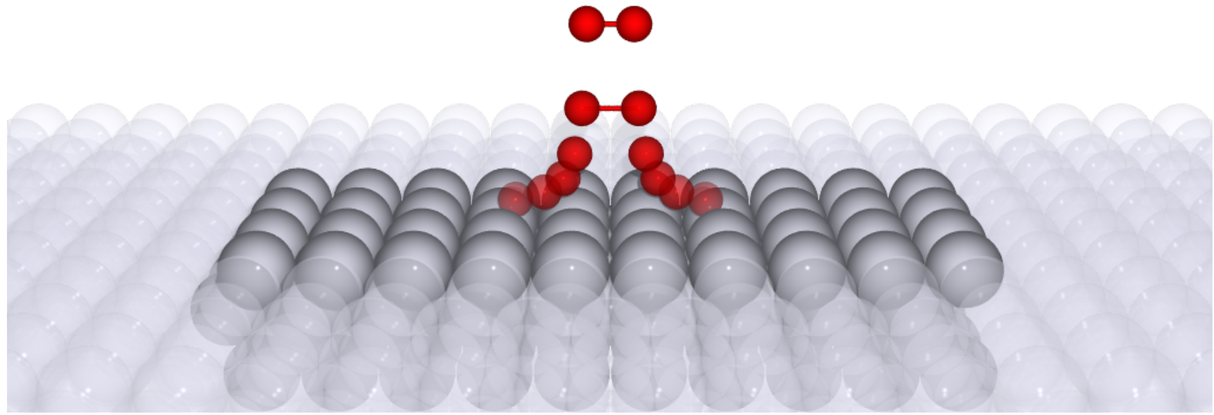
## Fast, error-proof, fun

When there's a task that can be done manually in 10 minutes but you find a way to automate it in 10 days

## Python libraries for atomistic materials modeling:

## ASE

- ASE - is an Atomic Simulation Environment written in the Python programming language with the aim of setting up, steering, and analyzing atomistic simulations.
- Good documentation with tutorials - Interfaces for most popular modeling simulation codes for density functional theory, molecular dynamics, etc
- Main features:
  - Atoms object for handling molecules/crystals
  - Read/write input files | Parse output files
  - Optimizers
  - Calculators
  - Visualization
  - Surface modeling



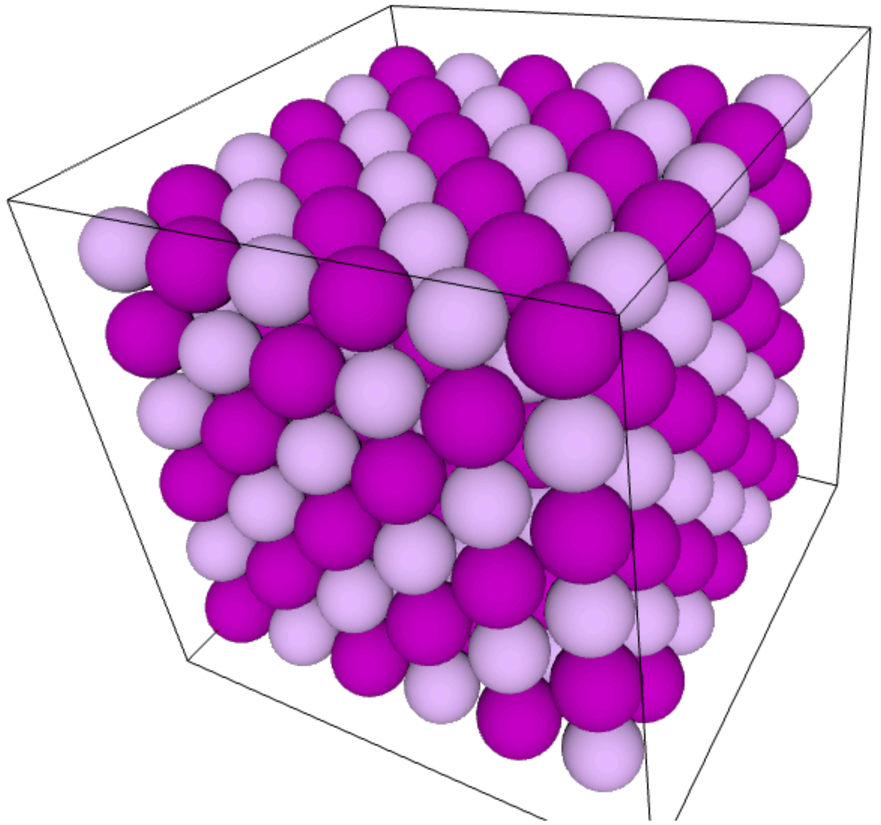
ASE documentation

## ASE minimum usage example

- read .cif file
- create supercell
- visualize
- save supercell
- more at the seminar

```
from ase.io import read, write
from ase.visualize import view
from ase.build import make_supercell

atoms = read('data/LiI.cif')
sc = make_supercell(atoms,
  [[3, 0, 0 ],
   [0, 3, 0],
   [0, 0, 3]]
   )
view(sc, viewer='x3d')
write('data/LiI_3x3x3.cif', sc)
```

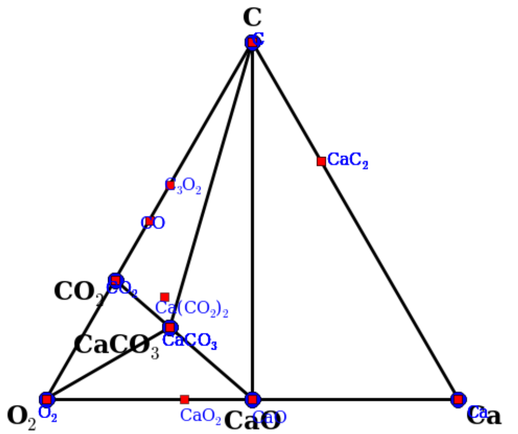


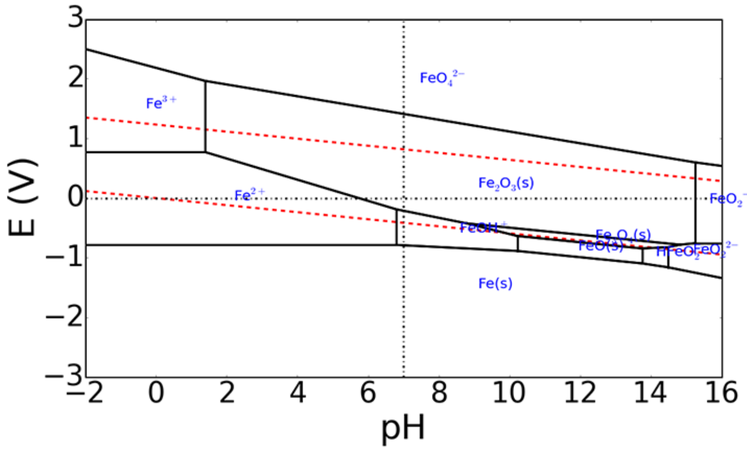
ASE documentation

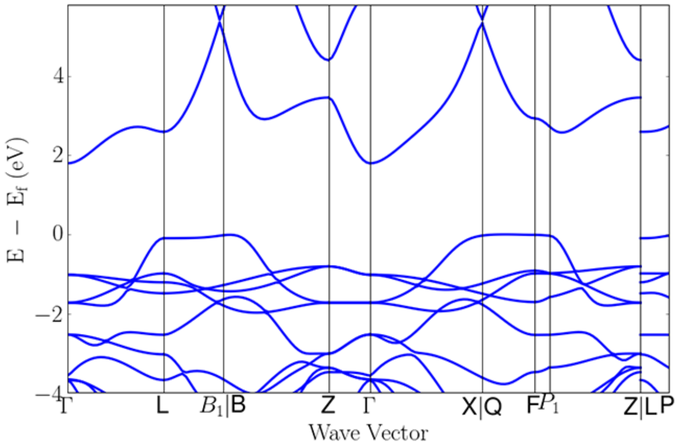
## Python libraries for atomistic materials modeling:

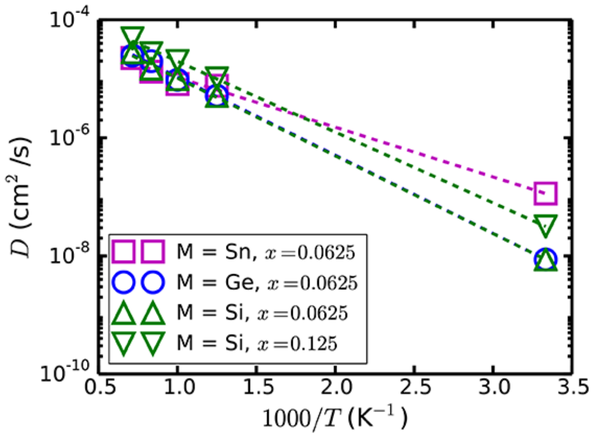
## Pymatgen

- Pymatgen (Python Materials Genomics) - a robust, open-source Python library for materials analysis
- Main features
- Highly flexible classes for the representation of Element, Site, Molecule, Structure objects.
- Powerful analysis tools, including generation of phase diagrams, Pourbaix diagrams, diffusion analysis, reactions, etc.
- Electronic structure analysis
- Integration with The Materials Project REST API (next lecture)

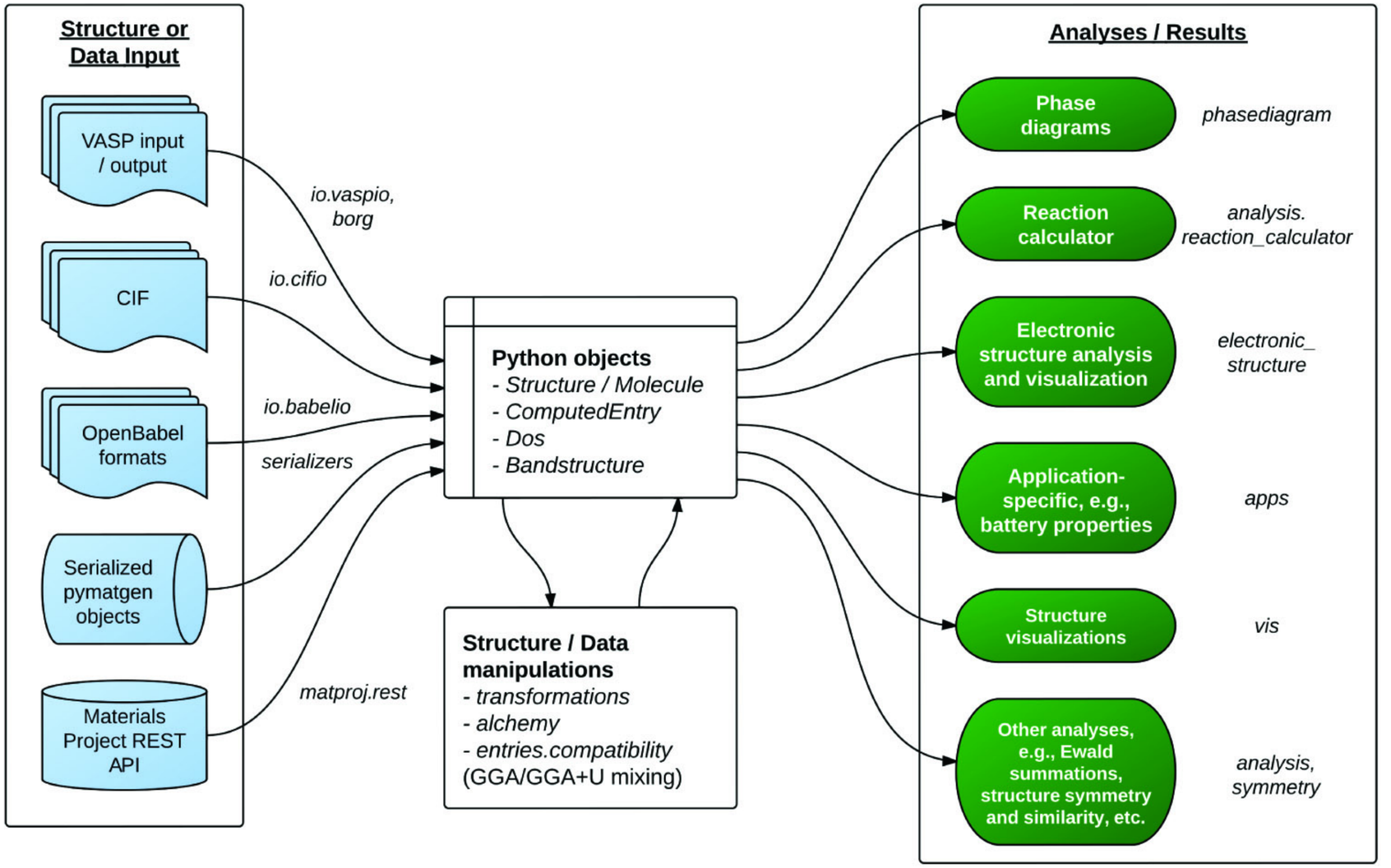


## Basic workflow with pymatgen



# Take home message

## Automation:

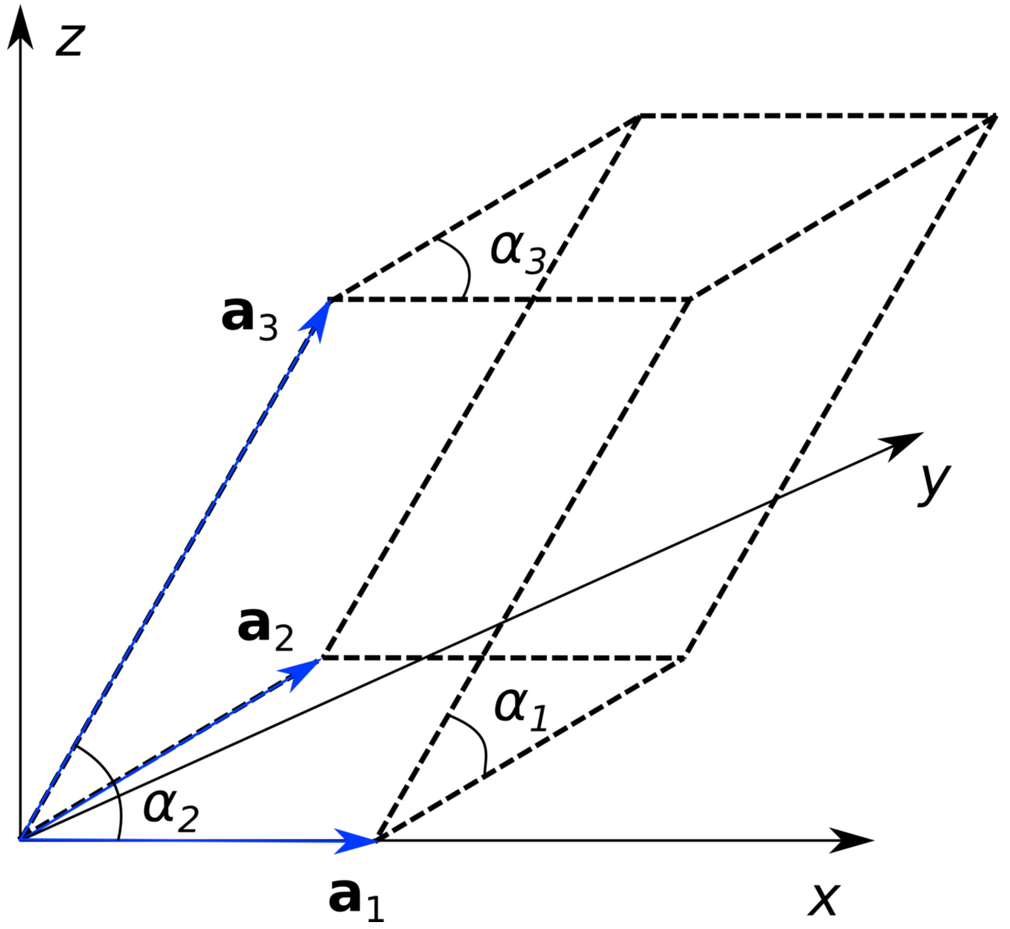
- saves your time
- gives you the opportunity (tools) to realize your ideas
- reduces number of mistakes (typos) made

# A few words about periodic boundary conditions before the start of the seminar

## Fractional coordinates:

- Crystallographic basis ($\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$) = basis vectors of the coordinate system
- Coordinate of an atom: $\mathbf{r}$ = (x, y, z)
- Fractional coordinate of the atom: (x/|$\mathbf{a_1}$|, y/|$\mathbf{a_2}$|, z/|$\mathbf{a_3}$|)

https://en.wikipedia.org/wiki/Fractional_coordinates



## There is a three dimensional periodicity in crystals = translational symmetry

- The smallest repeating unit, **unit cell**, describes the whole crystal
  - translation (basis) vectors (**a**, **b**, **c**)
  - coordinates of atoms in the unit cell {$\mathbf{r}_i$(x, y, z)}
- Any atomic position, **r**, in the crystal is given by $\mathbf{r}_i^{mnk} = \mathbf{r}_i + m\mathbf{a} + n\mathbf{b} + k\mathbf{c}$
  - m, n, k - integer numbers

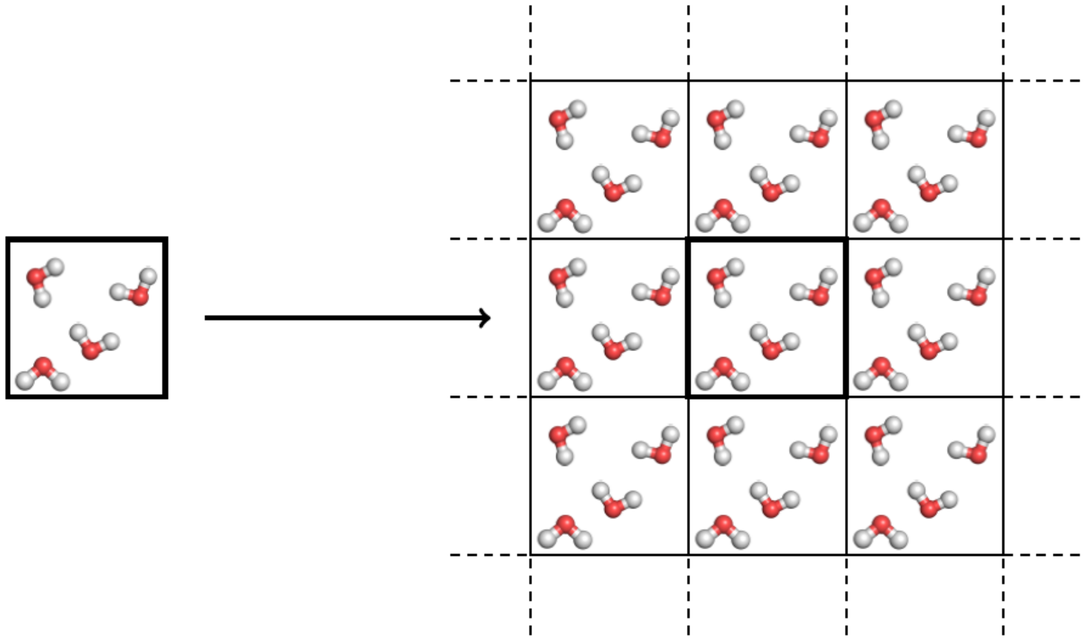


Image source

# Thank you for your attention!