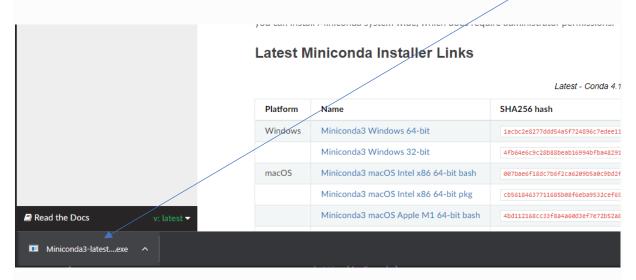
Step 1: Install conda

Download and install the version of conda for your operating system from http://conda.pydata.org/miniconda.html.

Platform	Name	SHA256 hash
Windows	Miniconda3 Windows 64-bit	1acbc2e8277ddd54a5f724896c7edee112d068529
	Miniconda3 Windows 32-bit	4fb64e6c9c28b88beab16994bfba4829110ea3145
macOS	Miniconda3 macOS Intel x86 64-bit bash	007bae6f18dc7b6f2ca6209b5a0c9bd2f28315415
	Miniconda3 macOS Intel x86 64-bit pkg	cb56184637711685b08f6eba9532cef6985ed7007
	Miniconda3 macOS Apple M1 64-bit bash	4bd112168cc33f8a4a60d3ef7e72b52a85972d588
	Miniconda3 macOS Apple M1 64-bit pkg	0cb5165ca751e827d91a4ae6823bfda24d22c398a
Linux	Miniconda3 Linux 64-bit	78f39f9bae971ec1ae7969f0516017f2413f17796
	Miniconda3 Linux-aarch64 64-bit	5f4f865812101fdc747cea5b820806f678bb50fe0
	Miniconda3 Linux-ppc64le 64-bit	1fe3305d0ccc9e55b336b051ae12d82f33af408af
	Miniconda3 Linux-s390x 64-bit	ff6fdad3068ab5b15939c6f422ac329fa005d56ee

For Windows, **make sure it is the Miniconda3 installer**, and simply double-click the exe file.



For Linux or Mac, go to folder in the terminal where the downloaded file is and type:

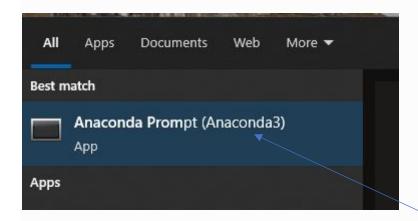
```
# If Mac
bash Miniconda3-latest-MacOSX-x86_64.sh
# If Linux
```

Step 2b: Create a conda environment

If you are working with many python packages, it is generally recommended you create a separate environment for each of your packages.

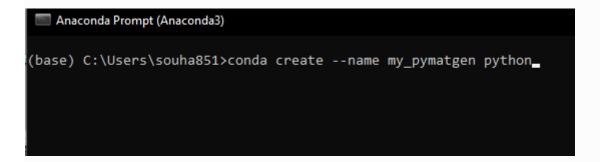
Windows:

search for the Anaconda prompt



Here it should say miniconda and not anaconda.

conda create --name my_pymatgen python
source activate my_pymatgen # OSX or Linux
activate my_pymatgen # Windows



Step 3: Install pymatgen

You can install pymatgen via conda as well via the conda-forge channel on Anaconda cloud:

conda install --channel conda-forge pymatgen

Step 4: Install jupyter notebook

Activate your environment

source activate my_pymatgen # OSX or Linux
activate my_pymatgen # Windows

Type:

conda install jupyter notebook

Step 4.5: Install jupyter notebook

Install mp_api

Type:

pip install mp_api

Install pycalphad

Type:

conda install -c conda-forge pycalphad

conda install -c conda-forge nbformat

Step 5: Connect jupyter notebook and test installation

pip install ipykernel

python -m ipykernel install --user --name="my_pymatgen" --display-name="My project (my_pymatgen)"

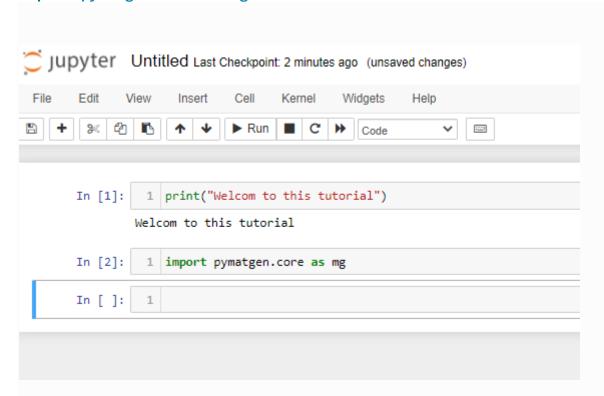
jupyter notebook

Now Jupyter notebooks will open in a new browser. It can look like this: 💢 jupyter Quit Logout Files Running Select items to perform actions on them. □ 0 - •/ ☐ ☐ 3D Objects 2 years ago ☐ ☐ Anaconda3 3 months ago □ Batteries 6 months ago ☐ Box Sync a year ago □ Contacts ☐ ☐ dagbok 7 months ago □ Desktop 5 hours ago For example, go to Desktop and create a new folder jupyter Rename directory Files Running Clusters Rename Move Enter a new directory name: ☐ 1 ■ / Desktop Thermodynamics tutorial ☐ clease-tutorial Cancel Rename ☐ Labreports □ Notebooks posters_essence ☐ ☐ Riman ☐ Thermodynamics-tutorial-1-main Untitled Folder Click new again and choose Python 3. A jupyter notebook will pop up where you can write code. Jupyter Untitled Last Checkpoint: a few seconds ago (unsaved changes) Logout Edit View Insert Cell Kernel Widgets Help Trusted Python 3 O **~** Welcom to this tutorial

Now, lets test if pymatgen works. Click on the plus and a new box will appear

Type:

import pymatgen.core as mg



If no warning or error pops up, it should work.

Test mp_api, type:

from mp_api.client import MPRester

If no warning pos up, you're good to go.

```
List of commands:

conda create --name my_pymatgen

conda activate my_pymatgen

conda install --channel conda-forge pymatgen

pip install mp-api

conda install -c conda-forge nbformat

conda install -c conda-forge pycalphad

pip install ipykernel

python -m ipykernel install --user --name="my_pymatgen" --display-name="My project (my_pymatgen)"

jupyter notebook
```