

## Instructions for running python

1. Navigate to <https://www.anaconda.com/> and download miniconda
  - a. This is an installer for a package manager called conda. Python is the programming language but there is a whole ecosystem including code editors, interactive notebooks and millions of packages. Packages are scripts that others wrote for you like for instance scikit-learn which is a package that includes a lot of machine learning tools. You will get to know all the different things in python over time.
  - b. Install miniconda
  - c. Installing the base python version from python.org is not recommended for beginners
  - d. If you are using one of the PCs in the PC room, you won't have sufficient rights to let conda run its scripts in the Windows command prompt. Type "conda install console\_shortcut" in the windows command prompt(Eingabeaufforderung) to get the Anaconda command prompt(if you installed anaconda instead of miniconda this will already be preinstalled). Open the Anaconda command prompt instead of the Windows command prompt.
2. Create a virtual environment. A virtual environment lets you build your own environment. This way you can avoid changing your whole system. Possibly incompatible packages/versions for different projects can be separated.
  - a. Type "conda create -n ml4chem" to create a new virtual environment ml4chem. This won't have any packages, so that we can get used to creating our own environment.
  - b. Activate the environment with "conda activate ml4chem".
  - c. Install a few basic packages: "conda install numpy", which install a powerful library for calculations with vectors, matrices, and tensors. "conda install notebook" to install Jupyter Notebook, a code editor, which lets you execute python commands step by step.
3. Open a jupyter lab notebook
  - a. Type "jupyter notebook"
  - b. Load the file 0\_Python\_Crashurs.ipynb into jupyter and run the individual cells
4. I recommend you use VisualStudio Code (not VisualStudio!) as an editor, while not using Jupyter Notebooks.
  - a. <https://code.visualstudio.com/>

If all of this fails and you happen to have a google account, you can also run a jupyter notebook on the google cloud here:

<https://colab.research.google.com/drive/1RSoFMl1lvYvzqP-dD5A-zmSc-fckSygb?usp=sharing>