



## Links to materials for preparing to the Spring School hands on tutorials

### Python

Machine Learning in Chemistry will utilize iPython Notebooks. Basic understanding of the Python language will enable focusing to the scientific content in the tutorials instead of the Python syntax. To get started, we recommend the following interactive tool for trying out Python:

<https://www.learnpython.org/>

You can also have a look at the [2017 Notebooks in here](#) (select Introduction to Machine Learning in Chemistry Notebook)

### Linux

In the School, you'll only need to be able to move around in the directory hierarchy (`cd`, `ls`, `pwd`), create directories, copy, rename, delete files (`mkdir`, `cp`, `mv`, `rm`), uncompress files (`tar`, `unzip`), edit files (any text editor, e.g. `gedit`, `nano`, `emacs`), look at file contents (`more`, `less`).

[https://www.csc.fi/web/training/-/linux1\\_sept2017](https://www.csc.fi/web/training/-/linux1_sept2017) (check the materials links)

<http://www.ee.surrey.ac.uk/Teaching/Unix/> (the first two topics is a good start, try also some editor)

[https://www.youtube.com/watch?v=uFPly\\_nGBMg](https://www.youtube.com/watch?v=uFPly_nGBMg) (sit back and watch)

[CSC Linux Cheat Sheet](#) (one page summary of most important Linux commands and then some)

### Gromacs

If you are new to Gromacs, but would like to participate in the Intermediate or Advanced tutorials, you can either work through the Basic tutorial from 2017 ([pdf](#)) ([tgz](#)), but this will require having access to Gromacs. Participating in the Basic tutorial in 2018 does not require prior knowledge of Gromacs.

### Turbomole (QC intermediate hands-on tutorial)

Please install the TmoleX 4.3 GUI on your laptop if you plan to take the intermediate QC tutorial.

<http://www.cosmologic.de/support-download/downloads/tmolex-client.html>

### NoMachine Remote graphics access to CSC servers

Please install the NoMachine 6.0 *Client* (not the *Desktop*): <https://www.nomachine.com/download-enterprise>

We recommend this for all remote work at CSC's server, note that if you don't have a CSC account, you won't be able log in yet. *Installation* requires administrative privileges, but the connection can be configured on-site at CSC.