

Module 2 Requirements

- Python (examples were tested on version 3.8.8)
- The following libraries should be installed:
 - numpy (examples were tested on version 1.19.2)
`pip install numpy`
 - torch (examples were tested on version 1.8.0)
`pip install --pre torch torchvision -f https://download.pytorch.org/whl/nightly/cu100/torch_nightly.html`
 - [torchani](#) (examples were tested on version 2.2)
`pip install torchani`
- [PyMOL](#) (Examples were tested on version 2.3.4) - An activation license for versions 2.x can be found in the module's folder: "pymol-edu-license.lic". If, for some reason, this license does not work, a new one can be downloaded from this website: <https://pymol.org/ep>, using the following credentials:
USERNAME: jun2021
PASSWORD: betabarrel
- Your favourite IDE (for this module I will use Visual Studio Code 1.54.3)