PHYMOL Training School 3:
Preparation for the workshop on properties

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For the workshop on molecular properties we will be using the VeloxChem software. It is crucial that you have completed the following installations *before* the workshop. If you run into problems, please reach out.

Installing Miniconda

All the programs and packages we need are available as `conda` packages. Install Miniconda following the instructions in this link (or find your own way).

Installing VeloxChem

OBS: If you already have an environment with VeloxChem from an echem workshop, please do carry out these steps anyway to have the latest build.

1. Create a directory somewhere on your laptop for the workshop files.
2. Download the file `phymol-ts3.yml` from this GitHub page and move it to the directory you just created.
3. If you have a Windows computer, open the `Anaconda Power Shell`; on Mac and Linux, open a normal terminal. In the terminal, navigate to the directory where the downloaded `.yml` file is and run the following command:
   `conda env create -f phymol-ts3.yml`
4. This creates a `conda` environment named `phymol-ts3` where VeloxChem is installed. You activate the environment with the command:
   `conda activate phymol-ts3`

Testing the conda environment

1. Download the file `testenv.ipynb` from GitHub and put it in the directory you created previously.
2. From the terminal/Anaconda Power Shell with the activated `phymol-ts3` environment open the file in Jupyter Lab with the command:
   `jupyter-lab testenv.ipynb`
3. In the `Kernel` drop-down tab click "`Restart Kernel and Run All Cells`". If the notebook runs without any error messages, you are good to go!