## **Prediction of molecular crystals structure.**

1. ssh to the account

**$ssh userXX@195.133.216.203**

where XX being the number sent to you in two digit format, e.g. number 3 corresponds to **user03**

1. Create new folder and cd into it:

**$mkdir EX\_Molecular  && cd EX\_Molecular**

1. Copy the files for example 23:

**$cp -r /opt/USPEX/uspex-2022.1-examples/EX37-3D-molecules\_H2O\_gulp/\*** ./

1. Open input.uspex file with vim editor.

**$vim input.uspex**

Optional.

Press **i** to enter the editing mode.

Press ESC to exit editing mode.

Type :wq to save changes and exit the editor

1. Open the job file with vim editor.

**$vim jobscript**

1. Load modules required for the calculations:

**$module load module load python/python39 uspex/uspex-2022.1 gulp/gulp**

1. Run the calculation:

**$sbatch jobscript**

1. Analyze the results (Individuals, gatheredPOSCARS, etc.).