These are the scripts used for the high throughput screening.

The main file is hts.sh. It has to be put in a folder that contains all the cif files and also all the other files necessary for running the calculations which are:

-template.param, template-dos.param (input files for castep).

-template.sh. template-dos.sh (template submission script for each single calculation)

You run the file by typing, in bessemer

*./hts.sh*

It will create a different folder for each MOF, which contains 2 folders: geom and MOF. The files template.param and template.sh are used to run the optimisation. Template-dos.param and template-dos.sh are used to run the dos (it will be automatic). More specifically, each of these files is going to be copied inside the corresponding folders, with the name of the MOF.

I advise to run no more than 30 MOFs per time.

In the same folder where you put the hts.sh file you can also keep the following files:

-printprob.sh 🡪 just informs you of what’s going on with each calculation, if there is any errors or if they are complete. When it says error unknown but it’s still running, very likely there is no error. The other possibilities are the most common errors: out of memory, convergence error for scf or for optimisation

-rerun-scf.sh 🡪 if there are convergence errors optimisation it will relax a bit the energies. It can be used once on the same MOF, hopefully after the first time you use it you fix the error. If you still have convergence errors after this, you need to figure it out on your own (or maybe give up)

-rerun-2.sh 🡪 is for a specific error that I made, but it should not happen I think

-search-oom.sh 🡪 it will stop the calculations that are giving out of memory errors, but then you need to fix the memory required manually in the .sh file for the MOF

At the very end you will have produced, in the main folder, a file called “result” In which the band gaps are written (this is created from the template-dos.sh file)