The script Complete\_list.py puts together all the data obtained from calculations and database.

Files needed:

-The file structural.xlsx is a file that contains different sheets and in each of the sheet the title indicates a specific structural property and the sheet contains a list of MOFs with that property. The property search was performed using the CCDC software ConQuest. Because the search of the structural criteria is a post calculations process, the file can be modified to add or remove properties.

-The file criteri.xlsx contains a sheet with a 4 different criteria that were used to screen the MOFs at the beginning of the project. Each column lists the criteria in the first row and all the MOFs with those criteria in the rest of the column.

-The file dosat\_15\_02\_22.xlxs is the file produced from the analysis of the results of the screening calculations. Every column lists MOF name, DoS at Fermi energy, band gap, DoS at VBM, DoS at CBM, type of structure. See ….

-The file metalli.xlsx contains a list of all the MOFs in the screening and the metals that they contain. It was obtained through the script ….

-The file metal\_density.xlsx contains a list of all MOFs in the screening and their cell volume, metal type, number of metals in a cell, metal density.

-The file all\_mofs\_reference.xlsx is used to get information on the number of criteria matched for the screening and other properties such as symmetry, temperature of synthesis, that were obtained through the use of ConQuest

-The file HSE\_results.xlxs was written as a result of the HSE calculations performed on the selected MOFs.

The script puts together all this information in an excel file ready to be analysed