Installation and use

This program is written to work with Python 3.6 or greater.
The required packages are located in the “requirements.txt” file and should be installed using pip.

First, set up a project folder with the following structure:
-Project folder
    -requirements.txt
    -peak_fitting.py
    -params_file.txt (will be created automatically with default parameters when the program is first run)
    -folder named “tga_files”
        -This folder should contain the .txt files corresponding to the TGA runs. There are three file formats available, currently (Q500/DMSM, TGA 5500, and a two column format without headers where temperature is in the first column, and mass is in the second)

Do this once:
Install python 3.6 following the instructions: https://www.python.org/downloads/

To install pip: https://www.liquidweb.com/kb/install-pip-windows/
(reach the command line by pressing Windows Key + r, type cmd into the text box, and press “run”)

Once python and pip are installed, using the command prompt, navigate to the folder where the navigate to the project folder (e.g. C:\TGA_experiments\carbon_nanotubes) and run the following command:
pip install requirements.txt

Do this for each new project folder:
Once the requirements have been installed, run the program by double clicking the peak_fitting.py file, or from the Command Prompt (in the project folder) run:
python peak_fitting.py

The first run in a project folder will create a default parameters file, and exit. Check the parameters and make changes as needed, keeping the same formatting as the automatically generated file (if format changes cause a problem with the params file, you can delete the old one, and the program will create a new one).
When there is a valid params file, running the program will perform a fit of every .txt file in the tga_files folder, so it’s important to make sure that these all have the same format (specified in the parameters), and that there are no other text files in that folder.
The program will create a folder “fits” in the project folder with fit results corresponding to the runs. The user can set a threshold for agreement between the integrated fit and experiment

above which more than just the single best (by BIC) fits are output, in this case a subfolder is created with fit results for that experiment.