Instructions on how to use `improved_calPE.py` to calculate the Parasitic Energy

1. To use **improved_calPE.py**, you will first have to install Cory's **pyIAST** program. Instructions on how to download the program can be found here: http://pyiast.readthedocs.io/en/latest/

   Link to the Github page: https://github.com/CorySimon/pyIAST

2. To run the program, enter the following command into the command line:

   ```
   ./improved_calPE.py coreDB.yml ABAVIJ coal IAST IAST
   ```

   Explanation of the input:

   `improved_calPE.py` → program to calculate the parasitic energy
   `coreDB.yml` → database
   `ABAVIJ` → name of the structure for which you want to calculate the parasitic energy
   `coal` → composition of the gas
   `IAST` → mixed-gas model
   `IAST` → save under which dictionary key

3. The output you get should look like something like this:

   ```
   ABAVIJ [914.4198, 2026.5, 333.0, 0.248214, 192.9399, 721.48,
   43.1682, 0.98971, 0.924254]
   ```

   Explanation of the output:

   `ABAVIJ` → name of the structure
   `914.4198` → parasitic energy in kJ/kg
   `2026.5` → pressure in Pa
   `333.0` → final temperature in K
   `0.248214` → final electricity loss (fraction)
   `192.9399` → final heat requirement in kJ/kg
   `721.48` → final compression work in kJ/kg
   `43.1682` → final mass of CO_2 produced in kg
   `0.98971` → final working capacity in mol/kg
   `0.924254` → final purity CO_2 (fraction)

Some things to keep in mind:

- The isotherm data should be put in the `ccsdata/`*`structure_name`* folder
  Eg. `ccsdata/ABAVIJ/`

- The temperature at which the isotherm data is calculated is automatically read from the filename `ccsdata/ABAVIJ/CO_2/`*`temperature`*`K.csv`
  Eg. `ccsdata/ABAVIJ/CO_2/300K.csv`
- Make sure to specify the name of the structure in the `coreDB.yml` file,

```
Structures:
  structure_name:
     Adsorbates:

Eg.
Structures:
 linker99_NH_linker96_CH2_pto_relaxed_trainB5:
     Adsorbates:
```