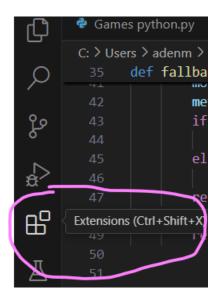
# Installing and running GAMESS to Excel reader

## By Aden Marines

### Fast tutorial:

- download Visual Studio code (look up, its popular)
  - go through typical "installing" process

#### -add extension:



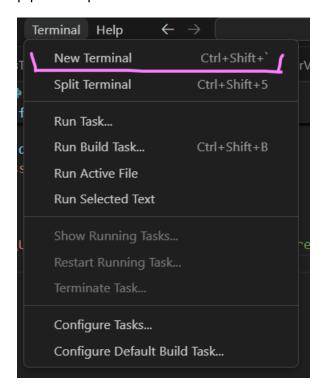
-search for "Python" and install



-open a terminal and install pandas:

Inside of terminal type:

pip install pandas



```
PS C:\Users\adenm\OneDrive\Documents\Python CH41e pip install pandas
Requirement already satisfied: pandas in c:\users\adenm\anaconda3\lib\site-packages (2.2.2)
Requirement already satisfied: numpy>=1.26.0 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (1.26.4)
Requirement already satisfied: python-dateutil>=2.8.2 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (2.9.0.post0)
Requirement already satisfied: pytz>=2020.1 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (2024.1)
Requirement already satisfied: tzdata>=2022.7 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (2023.3)
Requirement already satisfied: six>=1.5 in c:\users\adenm\anaconda3\lib\site-packages (from python-dateutil>=2.8.2->pandas) (1.16.0)
PS C:\Users\adenm\OneDrive\Documents\Python CH410>
```

-download attached "GAMEStoExcelReaderV2"

-Change filepaths for input and output folders.

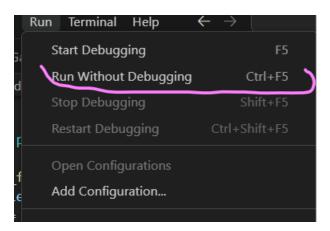
```
# === PATHS ===

input_path = Path(r'C:\Users\Public\gamess-64\outputs')
output_path = Path(r'C:\Users\Public\gamess-64\saved outputs\Python compiled csv')
output_path.mkdir(parents=True, exist_ok=True)
output_file = output_path / 'Gamess_summary.csv'

# === MAIN LOOP ===
```

This is the default directories, yours may be different. You can copy & paste your folder path by right clicking on the folder itself and "copy as path"

#### -run the code



#### -win

Output in Excel should look like this:

				_		-
molecule	force_field	basis	comp_met	bond_lengt	heat_of_fo	Total Energy (
C4H6	MMFF94	6-311ppG	Blyp	1.337955	NA	-155.931
C4H6	MMFF94	6-311ppG	RHF	1.337887	NA	-154.962
C6H8	MMFF94	6-311ppG	Blyp	1.445278	NA	-233.313
C6H8	MMFF94	6-311ppG	RHF	1.445278	NA	-231.874
HCl	Gaff	6311pp	AM1	1.099971	-11.3595	NA
HCl	Ghemical	6311pp	AM1	1.008097	10.5191	NA
HCl	MMFF94s	6311pp	AM1	1.305786	-24.4679	NA
HCl	MMFF94	6311pp	AM1	1.305889	-24.4666	NA
HCl	UFF	6311pp	AM1	1.375697	-22.4067	NA
He-neutra	MMFF94	6311ppG2	RHF	0	NA	-2.85998