

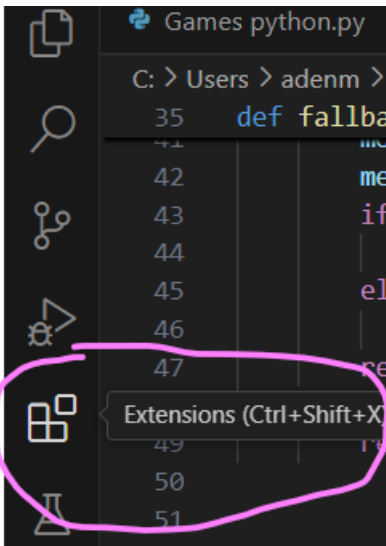
Installing and running GAMESS to Excel reader

By Aden Marines

Fast tutorial:

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

-add extension:



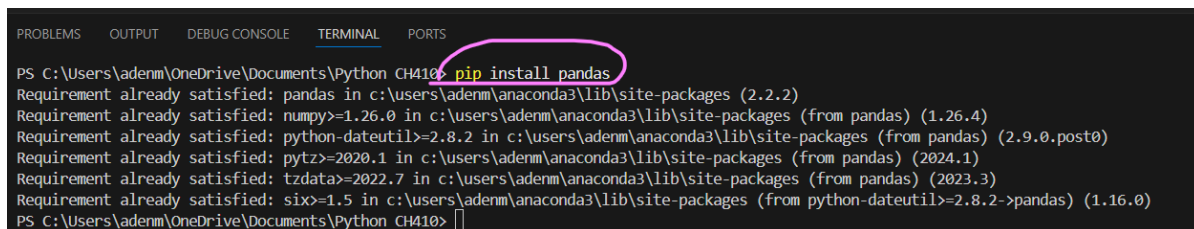
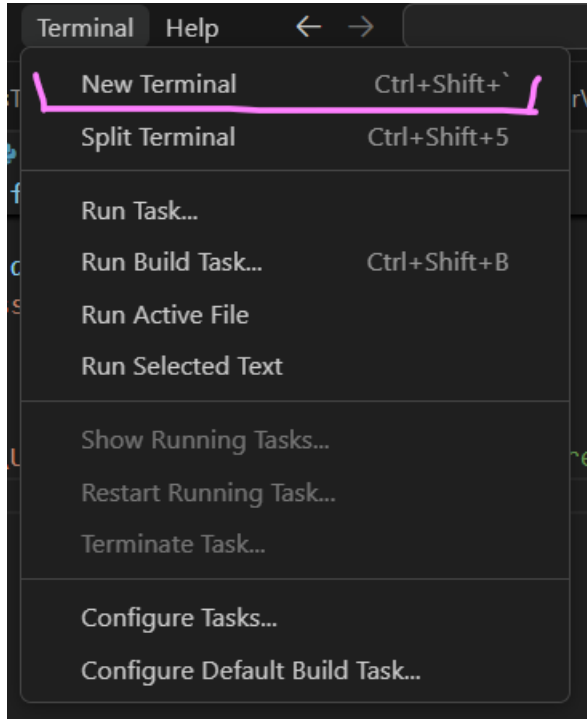
-search for “Python” and install



-open a terminal and install pandas:

Inside of terminal type:

pip install pandas



-download attached “GAMEStoExcelReaderV2”

-Change filepaths for input and output folders.

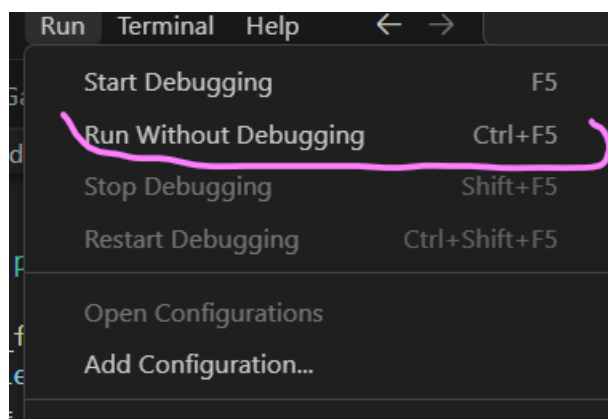
```
# === PATHS ===

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_length	heat_of_formation	TotalEnergy(kcal/mol)
	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
0	HCl	UFF	6311pp	AM1	1.375697	-22.4067	NA
1	He-neutral	MMFF94	6311ppG2	RHF	0	NA	-2.85998
2							