

https://github.com/DrZhiGong/HW4_CHEM179

HW4_CHEM179

Hi everybody, here is Zhi(Daniel) Gong speaking.

With the help of ChatGPT providing the Template to modify my codes and the open forums where there are too many wonderful tips for my coding life, most gratitude to my GSI Xiao, I have tried many times to access the right output of HO, HF, H2 for a long time.

And briefly speaking, I'd like to show some of the references I used.

Moreover, I tried to compile these codes in the Visual Studio 2022 Community WINDOWS and set the Armadillo package with the link I used. So please let me know if you meet some errors or other technical problems when you compiling these. DLL(/MDd) setup is what I used.

Just as you know, it needs quite a lot of works to access.

If you are confused, you can email me at zhigong@berkeley.edu or go to my office in Gilman Hall at UC, Berkeley.

Thank you for your love.

References:

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[5]<https://www.quora.com/What-is-an-intuitive-explanation-of-the-Hartree-Fock-method>

[6]<https://en.wikipedia.org/wiki/CNDO/2>

[7]<https://mattermodeling.stackexchange.com/questions/1540/how-to-calculate-the-fock-matrix-in-the-molecular-orbital-basis-pyscf>

[8]<https://mattermodeling.stackexchange.com/questions/1491/what-do-the-rows-and-columns-of-a-fock-matrix-represent>

[9]<https://mattermodeling.stackexchange.com/questions/4400/what-is-static-correlation-actually/4409#4409>

[10]<https://www.youtube.com/watch?v=IXaN7fzII7k>

[11]https://en.cppreference.com/w/cpp/error/logic_error

[12]<https://stackoverflow.com/questions/46489103/why-is-there-stdlogic-error>

[13]<https://cplusplus.com/forum/beginner/107516/>

[14]ChatGPT

[15]<https://github.com/XiaoLiu161147/Chem179-Spring2024>