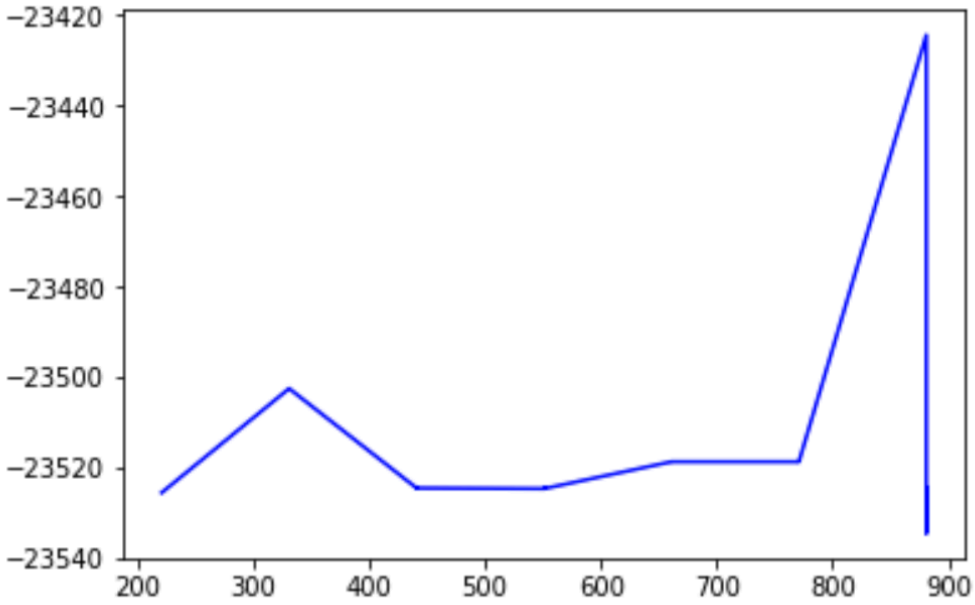
Summary of Final Goal

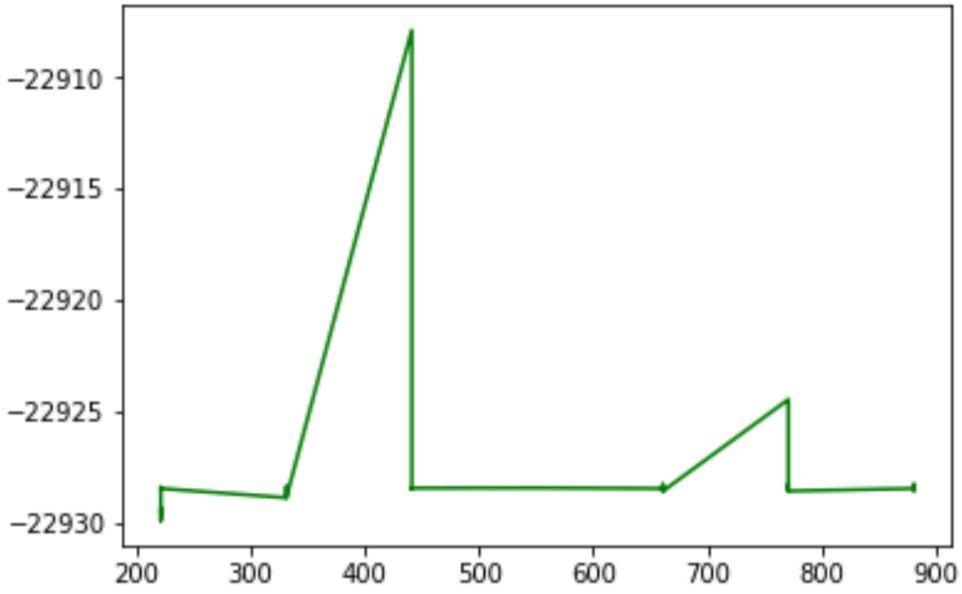
Robin Luo



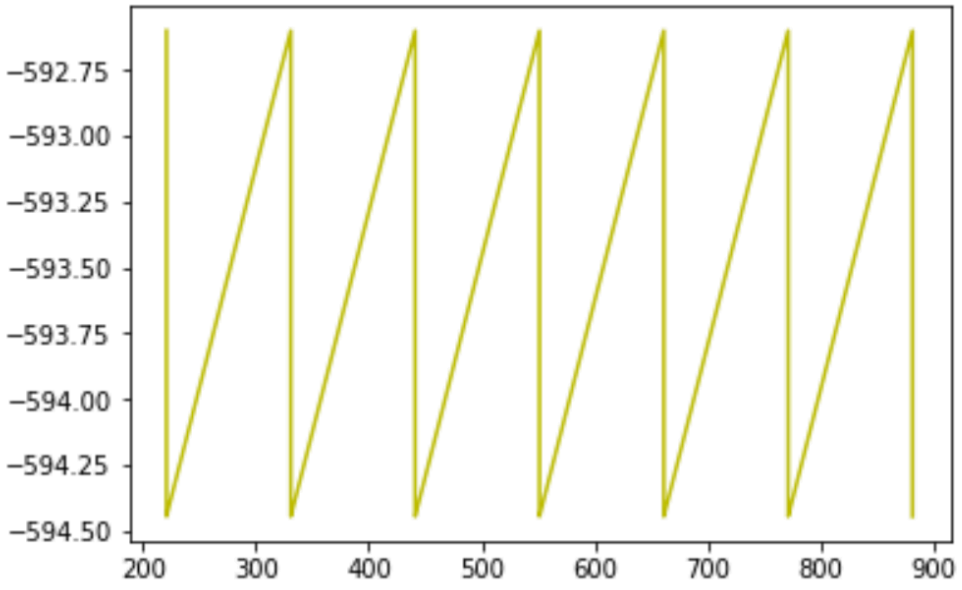
K-pts vs E_PtCO

Our results with the DFT calculation and PACE-ICE resulted in eV calculation is somehow similar in the past several years. The above graph is a result of plot for value of K-pts and E-PtCO. The below is the result of calculation and the code is attached in the autoFiles.

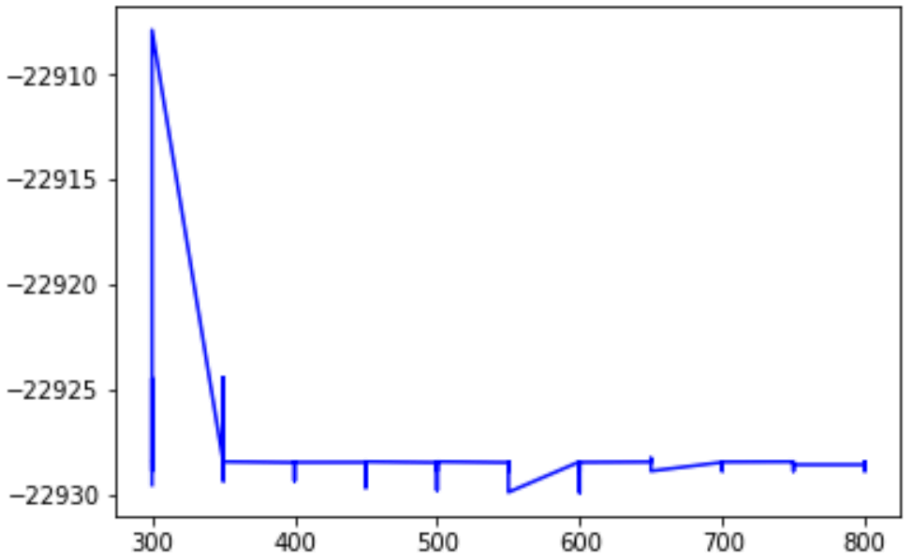
Graph of result:



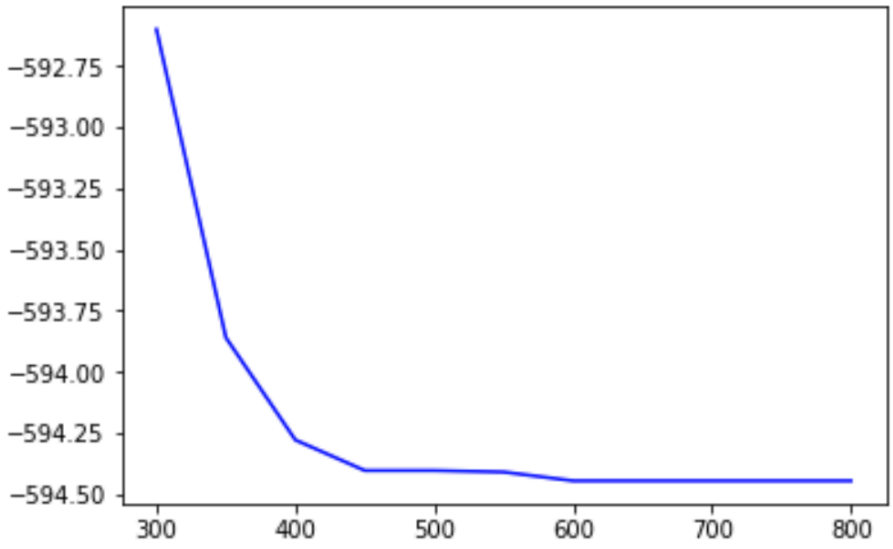
K-pts vs E-pt



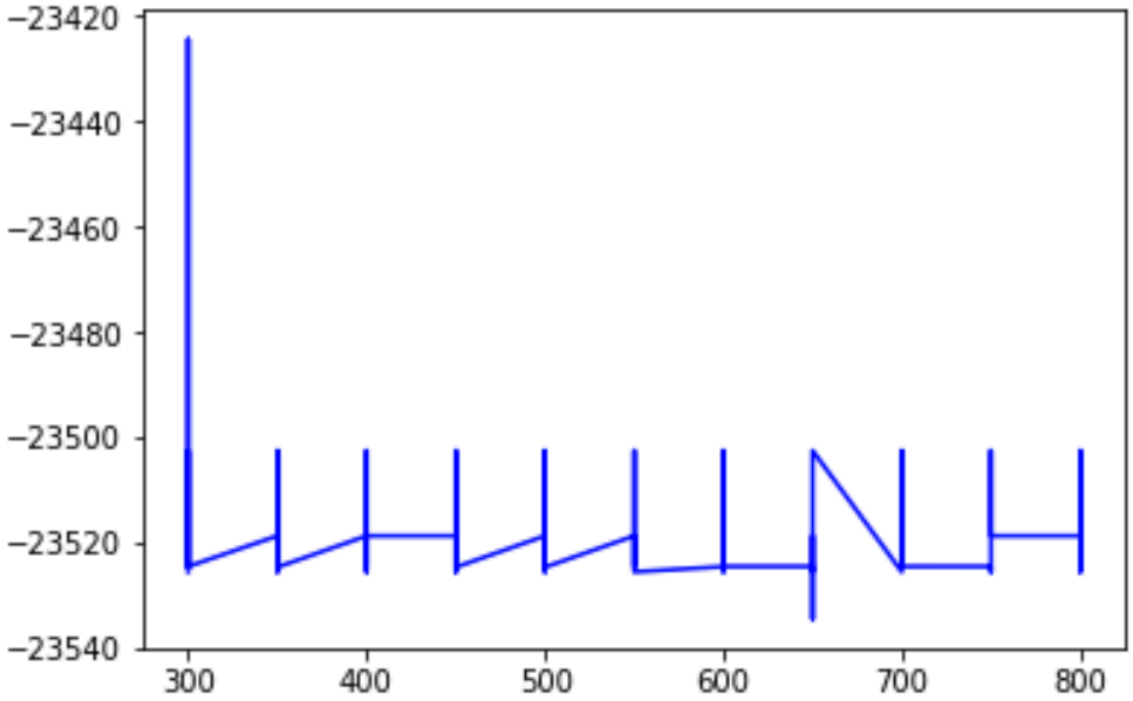
K-pts vs E-CO



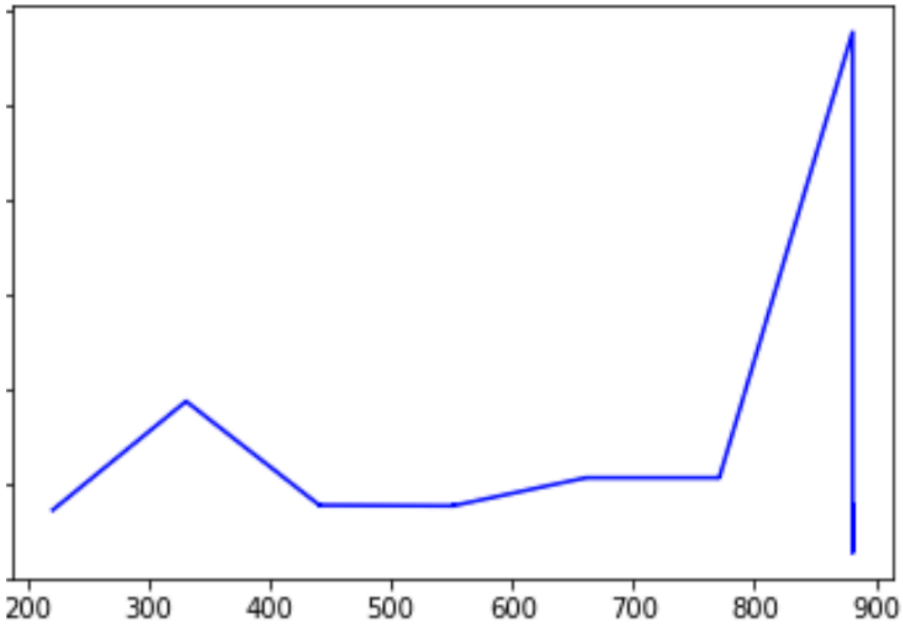
Plane-Wave VS E-pt



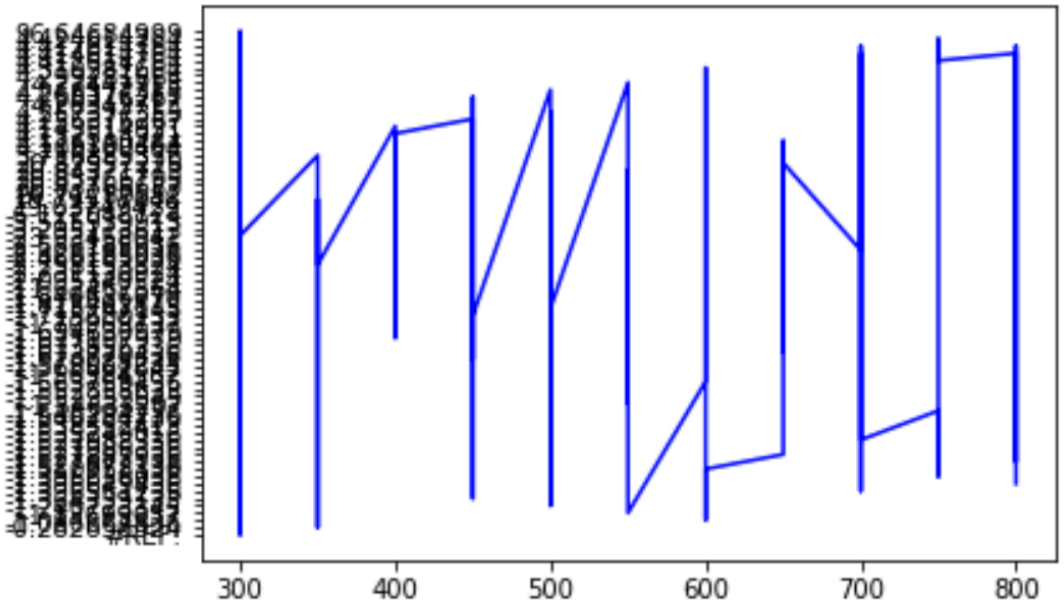
Plane-Wave VS E-CO



Plane-Wave VS E_PtCO



K- pts vs delta E_PtCO



Plane-Wave vs delta E_PtCO

data attach:

661	350	-23518.615		-22928.47059	-593.8592914	3.716885376
661	400	-23518.615		-22928.47059	-594.2769204	4.132514921
661	450	-23518.615		-22928.46959	-594.4017818	4.256376267
661	500	-23518.615		-22928.47059	-594.4017829	4.257377355
661	550	-23518.615		-22928.47059	-594.4078326	4.26342713
661	600	-23518.615		-22928.47059	-594.4436872	4.299281664
661	650	-23518.615		-22928.27941	-594.4436872	4.108100464
661	700	-23518.615		-22928.58893	-594.4436872	4.417614764
661	750	-23518.615		-22928.58393	-594.4436872	4.412614764
661	800	-23518.615		-22928.58893	-594.4436872	4.417614764
771	300	-23518.611		-22924.47104	-592.6016092	-1.538352413
771	350	-23518.613		-22924.47105	-593.8592914	-0.282658324
771	400	-23518.613		-22928.47959	-594.2769204	4.143514921
771	450	-23518.613		-22928.47959	-594.4017818	4.268376267
771	500	-23518.613		-22928.47959	-594.4017829	4.268377355
771	550	-23518.613		-22928.47959	-594.4078326	4.27442713
771	600	-23518.613		-22928.47959	-594.4436872	4.310281664
771	650	-23518.613		-22928.28541	-594.4436872	4.116100464
771	700	-23518.613		-22928.58393	-594.4436872	4.414614764
771	750	-23518.613		-22928.59393	-594.4436872	4.424614764
771	800	-23518.613		-22928.58393	-594.4436872	4.414614764

Instruction:

Minimal instructions for reviewers to understand the submitted files

1. the code of the automatic analyze of the energy.
    1. use cd go into dic which names as autoFiles
    2. check the file of baseFiles is satistified your requirment
    3. go back autoFiles dic and use python run the auto.py
    4. get the result
2. the result of the analyze
3. the graph of the analzye which include the surface and k-pt value with the three energy(delta total, CO, Pt111)

Links to any relevant files

https://www.sciencedirect.com/science/article/pii/S0039602818308124

https://aip.scitation.org/doi/abs/10.1063/1.440029

https://app.tettra.co/teams/medfordgroup/pages/calculating-adsorption-energies-a-crash-course

https://app.tettra.co/teams/medfordgroup/pages/automation-and-you-or-ushering-in-the-ai-apocalypse-for-fun-and-profit

contribution

In our group, we do the individual project and everyone give out there own result and then compare with each other and past several year result, I compare the result from the Hannah Li and Nick Ftatto and then change my data to get the correct of the result.

a self-assessment of which goals you achieved and why

1. Log in pace-ice
2. Successfully can use the Esspcro
3. Create molecules and slabs in several situation
4. Get a somehow good result of the calculation and get graph to visualization about the result.

Result:

From the result which we get from the calculation and we get the graph between each potential influence value of the energy. Finally we get the K-pts and surface both have a useful influence on the energy change. As the K-pts become large, the combined reaction energy will roughly increase and the Pt energy will increase first and then decrease. The highest point of reaction energy is 400 K-pts. For the CO energy change, the K-pts seem to do not have any influence.

For the change of surface, the Pt energy is no influence and for combine energy seems also no influence for the surface change. However, the CO energy is greatly negative

influence for the surface change. With the surface change larger, the energy change becomes lower.

The above all is the relationship between the three kinds of energy change and the influence value: surface and K-pts. Even though, I still think we have a lot of parts that can be improved. For example, we still can improve the accuracy of the data and become our automatic program be more smart and quick. The suggestions for my results and code are as follows:

1. Using the multi-thread to improve the efficiency of the atomic program, I think there we should use the one of the C/Java program to connect with our python code. Because the multithread of python code is actually not an actual multithread, it is a combination of several program parallel running. It can save some space but could not save the memory.

2. Using the C-store DBMS to store the resulting data and use the machine learning and data mining method to handle some dirty data. Actually, sometimes some of the results could not run out very well, which have the null value and wrong value, at this time we should clean the data. In this semester's research, because of lack of time, I did not use the data cleaning method to handle the data which we get.

3. Using the several plot tools and methods to get the visualization as a result, it would make our data more clear and understandable. It would let us find more useful relationship between the energy change and element change.