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I joined Dr.Martin's research group this fall quarter.I did not work but I learned a lot about the way research work is carried out.Working methods of both the groups gave me some ideas for work in the future.Not only did I learn about the research , but I also got an opportunity to learn about LATEX Syntax commands.I also gathered a little bit of knowledge about PYTHON language and its syntax.This experience also gave me an exposure about various methods used in reasearch work of other papers.I enjoyed my experience of working in Dr.Martin's group and would definitely love to work again further and contribute towards the research.

The two groups working on this research were the code group consisting of Son Nguyen and Santosh Kumar Vummidisingh and the research group consisting of Vusi Magagula, Ju Yi and Yi Li.Each of the groups had different goals to achieve.

Research Group:

The main aim of this group was to learn about Coupled Cluster Method with Single and Double Excitations and R12 Geminal terms method. After doing enough research and procuring information about these methods, they tried to compare these methods with the methods used in earlier research to find out which method is most cost effective and better.All the three methods were discussed in details with all notations very well explained.The Coupled Cluster Method(CC-Method) is a technique used for describing many body systems.In the RI method,it was concluded that this method could be used to reduce the computation cost of any Coulomb interaction Summation but not any exchange interaction summation.Mller Plesset Perturbation theory is a special application of Rayleigh - Schrödinger perturbation theory(RS-PT).It improves on the Hartree - Fock method by adding electron correlation effects by means of (RS-PT) to second,third and fourth order.This method is fast and reliable in its behaviour but at the same time it is not variational,thus making the estimate of correlational energy too large.After achieving their main aim,the next area of focus for research group is now to analyze the algorithm used for solving compact form of equations about cluster amplitudes.

Code Group:

The main aim of this group was to write a code which would generate the geminals and its symmetry group and then keep a track of all the geminal duplicates.They also generated all terms in the determinant of all the geminals and eliminated the ones which were of the same form.They used PYTHON language to write the code by which I learned some details about PYTHON syntax and certain functions used in the code.This code written by the group helped to find out the number of terms in geminals that were eliminated from the calculation so that the code is more cost effective.