

Project Title:

Relativistic Quantum Chemistry

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Ab initio calculations based on the first principle of quantum mechanics becomes more and more powerful with the increasing ability of computer power. Quantum chemistry programs are such tools for chemists to study the behaviors of molecules without experiments. Density functional theory makes the calculation of light elements containing molecules possible and fast. But there still exist a big challenge for the accurate calculation of heavy elements systems since relativistic effects is very important.

My research project is focus on the development of relativistic quantum chemistry methods to make the study of heavy elements systems more accurate and faster. Research will depend on the UTChem program which is developed by our group. Therefore, computational facility is necessary for our research, the super computer system will significantly accelerate our research progress.

In the past year of 2010, the UTChem program package was still under developing. A code was written for the newly developed two-component relativistic methods. But the program is still under debugging. Test calculations for small basis set and simple molecular system was done. For real applications the basis number is very large, therefore the program needs to be optimized for large scales calculations. Some of the programming and debugging was done in the RICC system.

However, RICC system is more suitable for large scale calculations. Our research goal is focused on heavy-element containing system, both theoretical and computational improvements are important. We will improve our program based on theoretical considerations, after that, calculation on interesting

system will be done.

In the future, we plan to apply the two-component methods including exact two-component method (X2C), Barysz-Sadlej -Snijders (BSS) and arbitrary order Douglas-Kroll -Hess (DKH) methods to the relativistic quantum chemical package UTChem with its two-component formalism. The benchmark four-component results will be compared for the justifying of accuracy. The scalar formation will be implemented into the existing developing version of Gaussian program, an extensive calculation on transition metal system and super heavy system will be done.

No achievement was made in the last year since both our theory and program were under developing. We thanks Advanced Center of Computing and Communication for the support of programming environments and achievement will be obtained in the future.