RICC Usage Report for Fiscal Year 2014

Project Title:

The development of new long-range DFT functional

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1. Background and purpose of the project, relationship of the project with other projects

In many body quantum chemistry calculations, the evaluation of two-electron integrals is the most time consuming bottle neck part. In particular, the acceleration of the evaluation of the Hartree-Fock exchange integrals is quite tedious, compared with that of the Coulomb integrals. Recent high applicability of hybrid density functional theory (DFT) functionals demands the improvement of the speed of the evaluation of the HF exchange integrations.

Recent our developed Gau-PBE hybrid functional has shown high performance on the solid state band gaps and reaction barrier height as well as quite improved low time cost for periodic boundary condition calculations.

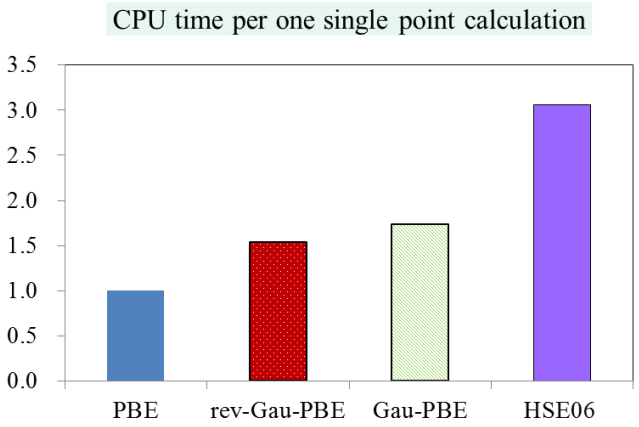
In this project, we proposed new efficient evaluation method for the HF exchange integrals of the Gau-PBE hybrid functional using multipole expansion of the Gaussian two-electron operator which is the two-electron Coulomb potential for Gau-PBE functional. In detail, we utilize the multipole expansion form of the Gaussian HF exchange as a screening scheme and try to decrease time cost for the HF exchange integrations, in particular, of Gau-PBE hybrid functional.

2. Specific usage status of the system and calculation method

In this project, we used RICC machine (mpc), specifically, for estimating the CPU time of new and old methods in order to confirm the superior efficiency of new evaluation method.

3. Result

As shown in figure, the previous Gau-PBE shows far less time cost than HSE06 hybrid functional which is world-widely used in the band gap calculations of the 7 popular semi-conductors, such as C, Si, SiC, BN, BP, MgO, and InN. In this time, we found that the Gau-PBE hybrid functional accelerated with multipole expansion scheme (rev-Gau-PBE) shows much less time cost than the previous Gau-PBE.



4. Conclusion

The rev-Gau-PBE needs only 1.5 times time cost of the PBE pure functional, which is an encouraging result and shows new evaluation scheme for Gaussian HF exchange integrals using multipole expansion is successful.

5. Schedule and prospect for the future

We expect this multipole expansion form for the Gaussian HF exchange integrals can be applied to general evaluation method for the integration scheme for Gaussian HF exchange. Therefore, we will actively develop the integration scheme using multipole expansion for the integrations with the Gaussian operator. In addition, we will apply the rev-Gau-PBE to the band-gap engineering technique for material systems.

Fiscal Year 2014 List of Publications Resulting from the Use of RICC

[Publication]

1. "Efficient evaluation method for Hartree-Fock exchange of Gaussian operator for Gau-PBE functional" J.-W. Song, M. A. Watson, and K. Hirao, *J. Chem. Phys.* submitted.
2. "Towards the Complete Range Separation of Non-Hybrid Exchange–Correlation Functional" Bun Chan, J.-W. Song, Y. Kawashima, and K. Hirao, *J. Comput. Chem.* in press.

[Oral presentation at an international symposium]

1. "Development of DFT functional applicable to large molecular and periodic systems" J.-W. Song CJK-WTCC-II conference (2015.01.23.), Kobe, Japan. [Invited]
2. "Efficient evaluation of short-range Gaussian attenuation Hartree-Fock exchange for periodic systems and large molecules" J.-W. Song, M. A. Watson, and Kimihiko Hirao, Molecular Electronic Structure (2014.09.03.), Amasya, TURKEY.
3. "長距離補正密度汎関数法による分子内電荷移動励起と分子間電荷移動励起の違いの解明" J.-W. Song and Kimihiko Hirao, The 17th Theoretical Chemistry Symposium (2014.09.23.), Nagoya, Japan.