Usage Report for Fiscal Year 2016

Project Title:

Development of new long-range corrected density functional theory and its applications

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

Long-range corrected (LC) DFT, where the HF exchange integral at long-range inter-electronic distance is included using a modified two-electron HF exchange Coulomb potential, clearly improves many problems of conventional DFT functionals. In detail, LC-DFT accurately reproduces frontier orbital energies and their gaps which, in contrast, conventional DFT methods underestimate. In addition, LC-DFT shows a 1/R behavior for charge-transfer excitation energies with respect to the separation (R) of the charges and this makes possible the application of LC-DFT to the study of intra- and inter-molecular charge-transfer excitations for large molecular systems.

Nevertheless, the evaluation of the long-range HF exchange integral has been the LC-DFT in terms of computational efficiency. Its high demand on computational resources prevents LC-DFT from being broadly applicable to real-sized systems. In contrast to the advancements in Coulomb integral evaluation, the calculation of HF exchange integrals is still quite time-consuming. At present, this obstacle prevents the application of hybrid functionals, including LC-DFT, to large systems, such as nano-materials, solid state materials, surface chemical systems, biomolecules, and so on.

In this project, we attempt to propose a new method to speed up the evaluation of long-range HF exchange integrals, which is of critical importance in the applications of LC-DFT to real-sized systems. We then hope to show that this new method reproduces the energies and properties of LC-DFT with shorter computational time for systems under the periodic boundary condition (PBC), as well as for large molecular systems.

2. Specific usage status of the system and calculation method

In this year, we didn't use either RICC or Hokusai machine due to busy schedule in new place and new position.

3. Result

In this year, we had no result since we didn't use any cpu time.

4. Conclusion

N/A

5. Schedule and prospect for the future

In the next year, we will perform adsorption energy calculations between molecule and metal surface. In addition, we will develop new method for acceleration of HF exchange.

6. If no job was executed, specify the reason.

In this year, the applicant's main affiliation was changed from RIKEN to Daegu university in Korea. Even though the applicant became a senior visiting scientist in RIKEN, new tasks in the changed environments didn't permit the applicant to proceed with researches proposed in the previous report.