

Project Title:

Long-range Corrected Density Functional Theory

Name : Raman Kumar Singh, Professor Takao Tsuneda, Professor Kimihiko Hirao
Affiliation: Next-generation Molecular Theory Unit
Advanced Science Institute Wako Institute

1. Background and purpose of the project, relationship of the project with other projects
2. Specific usage status of the system and calculation method
3. Result
4. Conclusion
5. Schedule and prospect for the future
6. If you wish to extend your account, provide usage situation (how far you have achieved, what calculation you have completed and what is yet to be done) and what you will do specifically in the next usage term.
7. If you have a “General User” account and could not complete your allocated computation time, specify the reason.
8. If no research achievement was made, specify the reason.

[Publication]

1. Raman K. Singh, Takao Tsuneda and Kimihiko Hirao "An Examination of Density Functionals on Aldol, Mannich and α -Aminoxylation Reaction Enthalpies" Theoretical Chemistry Accounts (2011) Submitted.
2. Raman K. Singh, Takao Tsuneda and Kimihiko Hirao "Long-range Corrected Density Functional Theory Study on Diels-Alder Reactions" (2011) to be Submitted.

[Proceedings, etc.]

If a publication does not contain the acknowledgement, please provide the reason for the missing of acknowledgement

[Oral presentation at an international symposium]

[Post Presentation]

1. Core Research for Evolutional Science and Technology (CREST) Symposium, 26th November 2010, Toyo University, Japan
2. Annual Meeting of Japan Society for Molecular Science, 14th Sept – 17th Sept 2010, Toyonaka Campus, Osaka University, Japan
3. 13th Annual meeting of theochem, 23 May -25 May 2010, Hokkaido University, Sapporo, Japan