Project Title:

Long-range Corrected Density Functionl Theory

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Present computational facility has made possible to perform computation from nano scale system to very large biologically active molecules to fetch a new perspective in science. *ab initio* quantum calculations handle micro system while ab initio molecular dynamic simulation deals large systems.

From the last two decades, Density functional theory (DFT) has been proved to give the properties of large system with reasonable good accuracy at low computational cost. This theory is also friendly with modern paralleling and linear scaling techniques. But in present time, it has been reported that DFT can not address weak interactions in a molecule properly. To overcome this problem, long range corrected DFT has emerged as a powerful tool which is pioneered by Hirao et al. Of late, we are attempting to develop and apply long range corrected DFT and time independent density functional theory (TDDFT) to deal with

(1) Enthalpy of Diels-Alder reaction
(2) Isomerazation energy of (CH)12 and other ring systems
(3) Dual fluorescence of DMABN
(4) Electron transfer process of photosynthesis of purple bacteria
(5) Initial process of TiO2 photo catalysis
(6) Photo induced phase transition of TTF-CA
(7) Metal free dye sensitized solar cells

If no research achievement was made, specify the reason.

I am in RIKEN since Jan 2010 and have started using RICC facilities right from the first week of Feb 2010. At present, no publication is in my hand and therefore I will present my reprint of publications and achievements in the next year.