Project Title:

Computation of frontier orbital energies for atoms and molecules using LC-DFT

Name: ○**Dr. Rahul Kar**

Laboratory at RIKEN: Advanced Institute for Computational Science, Kobe

1. Background and purpose of the project, relationship of the project with other projects: It has been known that the conventional density fucntionals could not predict the interaction energies for the noncovalent interactions such as hydrogen bond, van der Waals interactions. etc. Long-range corrected (LC) density functionals with reparametrized local response dispersion (LRD) method could be an alternative to calculate such interactions. Various noncovalent systems like the S66, S66X8, HBC6, NBC10 databases were chosen to optimize the parameters in LRD and tested on X40 database.
2. Specific usage status of the system and calculation method: All the computations were performed using Gaussian 09 software. We refitted the parameters in LRD in combination with LC-functionals and calculated the interaction energies. We used mostly 4 to 8 cores for our calculations.
3. Result: The new LRD parameters (in a.u.) were found: (i) κ=0.216, R_0=4.760, λ=0.228 for LC-BOP12+LRD and ii) κ=0.248, R_0=4.690, λ=0.229 for LCgau-BOP+LRD. We have calculated the interaction energy of the weakly bound intermolecular complexes compiled recently in the S66, S66X8, HBC6, NBC10 and X40 databases with the new parameterized LRD method with LC-DFT functional and compared with available wavefunction based methods and other density functionals. We found that the LC+LRD methods are well-balanced methods for the database reported with some exceptions in aliphatic-aliphatic type interactions. Test on the S66X8 database (with 8 non-equilibrium points) and the HBC6 and NBC10 database suggest that LC+LRD method with newly optimized parameters is a promising candidate for dealing such weak interactions not only at equilibrium geometries but also at non-equilibrium geometries..
4. Conclusion: LC fucntionals combined with LRD can be well-balanced and lower cost alternatives for weak interactions. However, further work needs to be done to test the parameters on different systems having weak interactions.

Fiscal Year 2013 List of Publications Resulting from the Use of RICC

[Publication]

"Long-Range Corrected Density Functionals Combined with Local Response Dispersion: A Promising Method for Weak Interactions" R. Kar, J-W. Song, T. Sato, K. Hirao. J. Comp. Chem. 2013, 34, 2353–2359