

Project Title:

Development of Long-range corrected density functional combined with local response dispersion method for weak interaction

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<p>1. Background and purpose of the project, relationship of the project with other projects: Description of non-covalent interactions such as hydrogen-bonding, van der Waals interaction has been one of the challenges for the density functional theory. Recently, our newly parametrized local response dispersion (LRD) combined with long-range corrected (LC) density functional theory has shown promising results in systems having weak interactions. However, the LRD method has scope for improvement. It can be combined with different LC functionals, and application of LC+LRD method to a wide range of systems having weak interactions can be tested.</p> <p>2. Specific usage status of the system and calculation method All the computations were performed using modified Gaussian 09 software. We used mostly 4 to 8 cores for our calculations.</p> <p>3. Result Earlier, the three LRD parameters κ, λ and R_0 were optimized for LC-BOP12 and LCgau-BOP functionals and tested for S66, S66x8, X40, HBC6 and NBC10 database. The dielectric model parameter λ was optimized for one value of l i.e., $l=1$ along with the other two damping parameters. Now we have tried to optimize the parameters for a generalized angular momentum with possible higher values of l. We optimized the dielectric model parameter with the other two damping parameters for LC-BOP12 and LCgau-B97 functionals. It was found that the RMSE=0.411 kcal/mol did not improve for LC-BOP12+LRD as compared to our previous results. Moreover, we found that</p>	<p>a negative value of damping parameter is observed in case of LCgau-B97 functional.</p> <p>4. Conclusion: The parameters in the modified LRD method were optimized for LC-BOP12 and LCgau-B97 functionals with the complexes of S66 database. Negative damping parameters suggest no physical meaning.</p> <p>5. Schedule and prospect for the future: The implementation of generalized LRD method need to be checked and tested for other long-range functionals.</p> <p>6. If no job was executed, specify the reason. Not applicable.</p>
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