The non-empirical versatile calculation method of the van der Waals interaction for isolated systems

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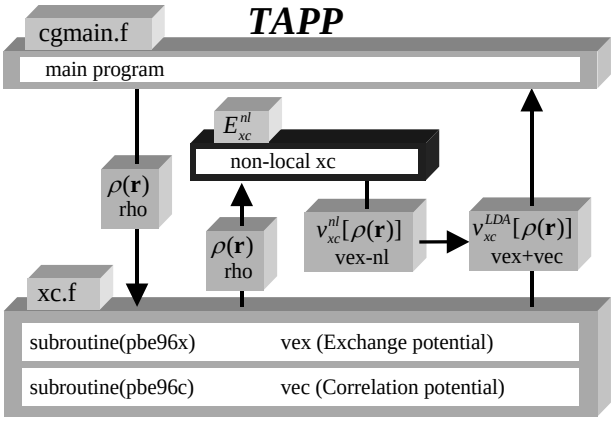
The local density approximation (LDA) cannot calculate the van der Waals interaction which significantly affects the non-local exchange correlation interaction. In order to cover this defect we develop a new method to calculate the van der Waals interaction for isolated systems. This method is designed to be absolutely non-empirical and to be able to attach into the various existing first principle electron state calculation routines utilizing LDA. (For example "TAPP") The starting point of this method is referred from the study by M.Dion *et al.*[*] They suggested the efficient method to calculate the van der Waals interaction utilizing the plasmon pole approximation. However an external parameter is referred in their approach to avoid large numerical calculation cost and therefore there are still difficulties in attaching into the non-empirical DFT-LDA method for various systems. Thus, in this study, we improve their method to be applicable to various isolated systems within small calculation cost and without any external parameters.



The dark shadow-casted block in the center of the right figure indicates the module code which is inserted into the self-consistent routine of DFT-LDA code "TAPP". Small blocks with allows indicates the flow of each variable used in TAPP while performing the self-consistent routine. As indicated in this figure, the only 'input' in our method is the total electron density $\rho(\mathbf{r})$ and the non-local exchange-correlation potential $v_{xc}^{nl}(\mathbf{r})$ as the 'output'. This makes us easy to insert our code into existing DFT-LDA codes.

At the poster session, we would like to introduce a concrete detail of our method and show some test results of isolated systems.

*M. Dion, *et al.* Phys. Rev. Lett. 92 (2004) 246401.