**Non-Covalent Interactions in Density Functional Calculations**

Yeil Kim, Suhwan Song, and Eunji Sim\*

*Department of Chemistry, Yonsei University, 50 Yonsei-ro Seodaemun-gu, Seoul, Korea*

\*E-mail: esim@yonsei.ac.kr

In this presentation, we introduce a practical method to correct various non-covalent interactions in density functional theory (DFT) using density-corrected DFT (DC-DFT)[1-2] and dispersion-corrected DFT (DFT-D). Various non-covalent interactions are considered an important role in the structure of materials and supramolecules. Despite DFT’s good balance between accuracy and computational cost, there still remain some challenges in DFT. To solve one of these problems, S.Grimme’s group developed the DFT-D3 method[3], an efficient silico-empirical method for non-covalent interactions with a predominance of dispersion. This correction can achieve better results in π-π interactions, hydrogen bonds, and some dispersion-dominant interactions using some standard benchmark sets. However, in the case of halogen bond, similar to hydrogen bonding in the aspect of dipole-dipole interaction, the result of DFT is worsened when dispersion correction is added. To classify the error in DFT, we employed the error classification of functional and density-driven errors. As a result, unlike other interactions, we found that halogen-bond is much more sensitive to density, which means density correction is necessary to cure the DFT error. By examining the B30 and the S22 datasets, we show that HF-DFT-D corrects the density and the dispersion simultaneously. The HF-DFT-D method provides more accurate results for non-covalent interactions, whether errors in standard DFT calculations are due to static or van der Waals forces.

1. M.-C. Kim, E. Sim, and K. Burke, Phys. Rev. Lett., 111, 073003 (2013)
2. A. Wasserman, J. Nafziger, K. Jiang, M.-C. Kim, E. Sim, and K. Burke, Ann. Rev. Phys. Chem., 68, 555-581 (2017)
3. S. Grimme, J. Antony, S. Ehrlich, and H. Krieg J. Chem. Phys. 132, 154104 (2010)