Analysis of the changes in electronic structures due to intermolecular interactions by using the difference of density matrices

Daisuke Yamaki

Research Organization for Information Science and Technology (RIST)
1-5-2, Minatojima-minami-machi, Chuo-ku, Kobe 650-0047 Japan

The size of molecules calculated by molecular orbital (MO) theory is becoming huge with the development of computation power and algorithms. To compare between a huge molecule and another similar reference molecule is difficult, because it is practically impossible to use the conventional MO-analysis that investigates the subtle difference between two sets of MOs for huge molecules. To overcome this situation, previously, we proposed analysis methods that use natural orbitals (NOs) of the difference density matrix between a target molecule and a reference molecule, which may have different numbers of electrons [1].

In this paper, we analyze the changes in the electronic states due to intermolecular interactions, e.g. hydrogen-bond interaction and van der Waals interactions, by using our methods (as shown in Figure 1), and discuss the applicability of our methods.

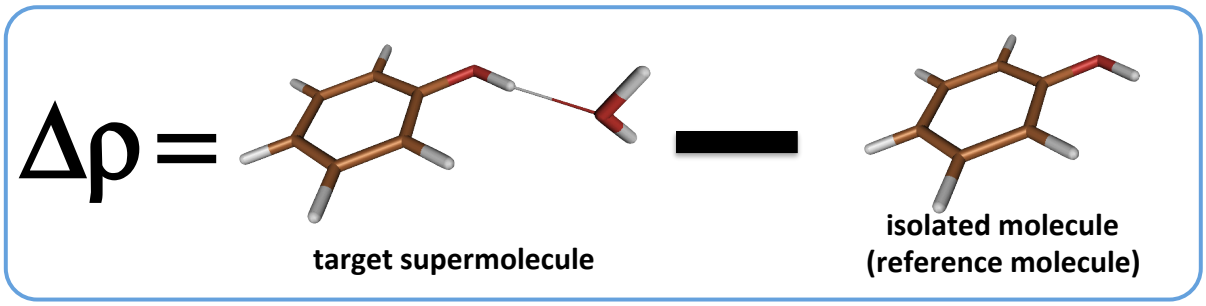

Figure 1 **Comparison of phenol-water complex with the isolated phenol molecule. The change of the electronic structures induced by the intermolecular interaction can be extracted by our methods.**

[1] D. Yamaki, Mol. Phys. **113**, 342 (2015). (DOI: http://dx.doi.org/10.1080/00268976.2014.951702)