

Difference density matrix analysis of epigenetic chemical modifications

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Epigenetic chemical modifications, such as DNA methylation and histone modifications play central roles in many types of epigenetic inheritance. The DNA modification, 5-substitution of methyl groups to cytosine residues in CG sites, can change the activity of a DNA segment without changing the sequence. The modification of histone proteins (acetylation, methylations, etc) affects gene expression. The relationships between these modifications and the changes of electronic states are interesting. In this study, we perform *ab initio* calculations for model molecules of modified/reference DNA and histone proteins, and compare them by using Difference Density Matrix Analysis (DDMA) method previously we proposed (as shown in Figure 1). This method utilizes natural orbitals (NOs) of the difference density matrix between the modified and reference molecules, which may have different numbers of electrons [1]. We analyze the changes of electronic states due to epigenetic chemical modifications.

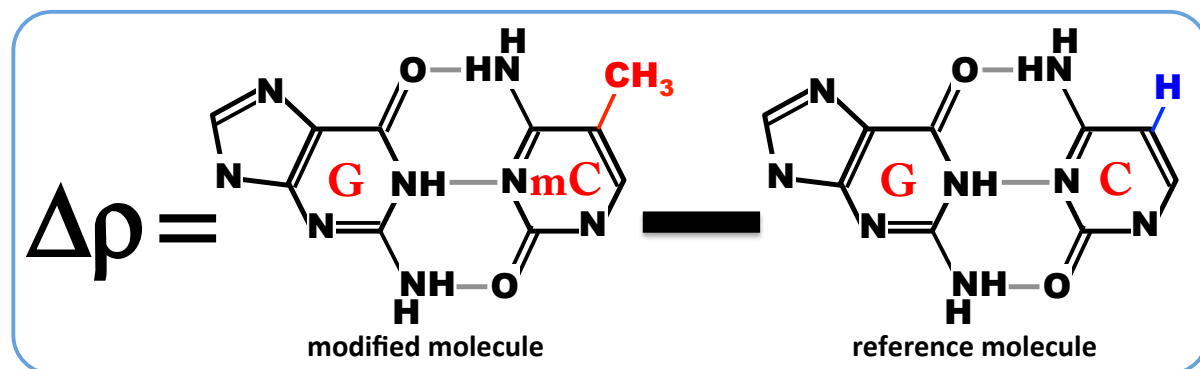


Figure 1 Comparison of a modified complex (GmC) and the reference complex (GC). The change of the electronic structures induced by the methylation can be extracted by Difference Density Matrix Analysis method [1].

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