

DNA – Protein interaction in the nucleosome system

Attila Bende^{1,2}, János J. Ladik²

¹ Molecular and Biomolecular Physics Department, National Institute for R&D of Isotopic and Molecular Technologies, Str. Donath 65-103, Cluj-Napoca RO-400293, Romania

² Chair for Theoretical Chemistry and Laboratory of the National Foundation for Cancer Research, Friedrich-Alexander-University-Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

The interaction between the negative side chain of DNA and the positive side amino acids of histone protein have been characterized by Hartree-Fock and second order Møller-Plesset perturbation theory level using the triple- ζ basis set with polarization functions in the framework of the two-layer ONIOM method [1]. The strength of the intermolecular interaction and the magnitude of the charge transfer between the DNA and the histone protein is discussed considering the presence of different positive (K^+ , Mg^{2+}) [2] and negative ions (Cl^-) [3] as well as water molecules. The role of the ions on the stability of the nucleosome systems and the possible consequences of the DNA unwrapping from the histone are widely discussed.

[1] A. Bende, F. Bogár and J. Ladik, *Chemical Physics Letters*, 437:117-119, 2007.

[2] A. Bende, F. Bogár and J. Ladik, *Chemical Physics Letters*, 463:211-213, 2008.

[3] A. Bende, F. Bogár and J. Ladik, *Chemical Physics Letters*, 525 - 526, 115 - 119 2012.