Quantum Theoretical Investigation to Explain the Onset of Cancer

János J. Ladik

Chair for Theoretical Chemistry and Laboratory of the National Foundation for Cancer Research,
Friedrich-Alexander-University-Erlangen-Nürnberg,
Egerlandstr. 3, 91058 Erlangen, Germany. E-mail: Janos.Ladik@fau.de

The stereostructure of DNA was established by Watson and Crick based on the X-ray investigations of Wilkins in 1953. Since that time with the refinement of the X-ray technique Richmond and Luger have given a more refined structure of DNA and the 8 nucleoproteins in the nucleosomes (particles in the cell nucleus from which the chromatins are formed) in 1997. Using this structure large scale quantum theoretical investigations have been performed using the *ab initio* HF crystal orbital method in its LCAO form. In the calculations besides the translation also the 36° rotation was simultaneously taken into account. This work was started from a single nucleotide (base with sugar and phosphate and surrounding water and Na^+ ion). The calculations were extended to periodic nucleotide stacks, stacks containing a base pair periodically repeated and in an approximate way to periodic two different nucleotide pairs. Using the obtained band structures with the help of the so-called deformation potential approximation the hole mobilities of the mentioned systems were calculated. Since, previously it was shown that chemical carcinogens and radiation hits act not only locally, but with the aid of different mechanisms in which solitons (non-linear quasi particles) play a central role, but also quite far from their original point of interaction with DNA. If a carcinogen activates in this way an oncogene through m.RNA and the occurrence of a protein (oncoprotein) at an unexpected place and time this can disturb the self-regulation of the cell. This cell then can become into another stationary state (so-called precancerous state). Since there is no contact inhibition between cancerous cells, the transition of normal cells into precancerous ones can dissipate easily and therefore a tumor can develop. The effect of a radiation hit on DNA can break one strand of the double helix. If a second hit occurs its effect can propagate with the help of the same mechanisms as in the case of carcinogens, to the site of the first hit and that causes a break of the double helix. This causes a loss of genetic information including the loss of the so-called antioncogenes. Finally, it should be mentioned that despite the large progress of the biological and chemical aspects of carcinogenesis without the understanding the physical and physico-chemical side of cancer development, it will be very difficult to find methods for its cure. This was most recently pointed out by the National Cancer Institute of NIH.