

Electronic structure of DNA revealed for the first time

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Utilizing a technique that combines low temperature measurements and theoretical calculations, Hebrew University of Jerusalem scientists and others have revealed for the first time the electronic structure of single DNA molecules.

The knowledge of the electronic properties of DNA is an important issue in many scientific areas from biochemistry to nanotechnology -- for example in the study of DNA damage by ultraviolet radiation that may cause the generation of free radicals and genetic mutations. In those cases, DNA repair occurs spontaneously via an electronic charge transfer along the DNA helix that restores the damaged molecular bonds.

In nano-bioelectronics, which is the advanced research field devoted to the study of biological molecules (to produce electrical nanocircuits, for example), it has been suggested that DNA, or its derivatives, may become used as possible conducting molecular wires in the realization of molecular computing networks which are smaller and more efficient than those produced today with silicon technology.

The knowledge that has been acquired in this project, say the researchers, may also be relevant for current attempts to develop new sophisticated, reliable, faster and cheaper ways to decode the sequence of human DNA.

The research, published in the prestigious journal *Nature Materials*, is a result of an international collaboration. The research was conducted by

Errez Shapir and coordinated by Dr. Danny Porath at the Department of Physical Chemistry and Center for Nanoscience and Nanotechnology at the Hebrew University and by Dr. Rosa Di Felice at the S3 Center of INFN-CNR in Modena, Italy. Also collaborating in the project were Prof. Alexander Kotlyar at Tel Aviv University, who synthesized the molecules, the CINECA supercomputing center in Italy, and Prof. Gianaurelio Cuniberti at the University of Regensburg, Germany.

In their work, the researchers were able to decode the electronic structure of DNA and to understand how the electrons distribute into the various parts of the double helix, a result that has been pursued by scientists for many years, but was previously hindered by technical problems.

The success of this project was finally achieved thanks to collaboration between experimental and theoretical scientists who worked with long and homogeneous DNA molecules at minus 195 degrees Celsius, using a scanning tunneling microscope (STM) to measure the current that passes across a molecule deposited on a gold substrate. Then, by means of theoretical calculations based on the solution of quantum equations, the electronic structure of DNA corresponding to the measured current has been obtained. These results also suggest an identification of the parts of the double helix that contribute to the charge flow along the molecule.

Source: The Hebrew University of Jerusalem

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