

Anatomy of Base Pairing in DNA

by Interacting Quantum Atoms

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The anatomy of bond energy for supramolecular interaction in base pairs of DNA was described in the light of theory of interacting quantum atoms (IQA) within the context of quantum theory of atoms in molecules (QTAIM)[1]. The interplay of individual physically meaningful energy components involved in three stages of bond formation process (structural deformation, electron density preparation, and intermolecular interaction) as well as assessment of electron sharing in the fragment[2] was studied.

We recognized that for the neutral base pairs the variation in the kinetic energy and electrostatic contribution to the bond energy are rather negligible, but the main source of bond energy was the exchange-correlation energy component. It can also be demonstrated that the contribution of the exchange-correlation energy component into the bond energy can be recovered by including atoms that are formally assumed to be hydrogen bonded. In contrast, to recover the electrostatic energy component of interaction one must consider both the short- and long-range contributions. This knowledge can be used for designing artificial DNA bases for various purposes including chemical biology and nanotechnology.

[1] R. F. W. Bader Atoms in Molecules. A Quantum Theory. Oxford University Press, New York, 1990.

[2] C. Foroutan-Nejad, Z. Badri and R. Marek, Phys. Chem. Chem. Phys., 2015, 17, 30670–30679