Effect of the Van-der-Waals and intramolecular forces

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In modern microelectronics, nanobiotechnology, nanorobots increasingly have being used both organic biomacromolecules and fragments, as nucleotides, peptides, DNA, and inorganic elements, like as metallic nanoparticles, carbon nanotubes.

The charge transfer in such heterogeneous systems to a large extent has to determined by the conformational changes of biological fragments. In studying the properties of these complex nanoparticles one of the effective tool is a hybrid method of molecular dynamics simulation, combining molecular-mechanical and quantum-mechanical approaches.

The above mentioned article devoted to the study of the interaction of the nucleotide chains (NC) and peptides, as well as RNA, DNA molecules, with metallic nanoparticles (NPs) in a matrix of carbon nanotubes (CNT) by the hybrid classical and quantum chemistry molecular modeling methods. The work is extremely important.

The tertary system NC-NPs-CNT represents a great interest in modern nano-bio-technologies, for the design of the electronic disgnostic tools, in drug delivery inside living cells, so on.

More information: M.A. Khusenov et al, On Correlation Effect of the Van-der-Waals and Intramolecular Forces for the Nucleotide Chain - Metallic Nanoparticles - Carbon Nanotube Binding, *The Open Biochemistry Journal* (2016). DOI: 10.2174/1874091X01610010017

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