

Effect of the Van-der-Waals and intramolecular forces

May 6 2016

In modern microelectronics, nanobiotechnology, nanorobots increasingly have been 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 be determined by the conformational changes of biological fragments. In studying the properties of these complex nanoparticles one of the effective tools 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 tertiary system NC-NPs-CNT represents a great interest in modern nano-bio-technologies, for the design of the electronic diagnostic 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](https://doi.org/10.2174/1874091X01610010017)

Provided by Bentham Science Publishers

Citation: Effect of the Van-der-Waals and intramolecular forces (2016, May 6) retrieved 1 July 2024 from <https://phys.org/news/2016-05-effect-van-der-waals-intramolecular.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.