سیویلیکا - ناشر تخصصی مقالات کنفرانس ها و ژورنال ها
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عنوان مقاله:

DFT/NBO Analysis of interaction between Nonsteroidal Anti–Inflammatory Drugs (NSAIDs) and Nanoadsorbents

محل انتشار:

نهمین کنفرانس بین المللی علوم و توسعه فناوری نانو (سال: 1401)

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خلاصه مقاله:

Various types of nanotubes have been studied as drug carriers all over the world. They can be used for drug delivery to release drugs wherever it is needed to prevent their side effects.For this Aim, in this work the interaction between Carbon Nanotube (۷,۰) and some Non-Stroidal Anti–Inflammatory Drugs (NSAIDs) such as Aspirin, Ibuprofen and Naproxen has been investigated. The Density Function Theory (DFT) calculations have been performed by Beck, three-parameter, Lee-Yang-Parr (B۳LYP) method and standard ۶-۳۱G(d) basis set for full optimization of complexes. The Natural Bond Orbital (NBO) analysis and frequency calculations have been also performed for all structures using B۳LYP method and the standard ۶-۳۱G(d) basis set in ۲۹۸K. All calculations were performed in gas phase, water and CCl۴ solvents. According to the results, all complex between Carbon Nanotube and the mentioned drugs are performed in all ۳ phases, Thermodynamically. NBO calculations have shown the existence of hyper conjugative effect in all structures which is made by overlapping between Lone pairs of Oxygen in drugs and * or * orbitals of Nanotube. Also, HOMO-LUMO energies and their relative properties as well as ESP and ED maps shows more reactivity and electron density in CNT parts of all coplexes.

کلمات کلیدی:

NSAIDS, Density Functional Theory, Carbon Nanotube, ESP, NBO, electron density, HOMO-LUMO.

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