Physico-chemical nanomaterials science

Vibrational spectra of acetaminophen-cholesterol system: DFT calculations

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The infrared and Raman spectra of the system composed of acetaminophen and cholesterol molecules were calculated using the density functional theory (DFT). The calculations were performed at the B3LYP/6-31G(d,p) and the B3LYP/6-311G(d,p) level of DFT theory. It is known, that oxidative modification of the low-density lipoprotein (LDL), which is the major carrier of cholesterol in blood stream, contributes to the development of atherosclerosis [1]. Acetaminophen, also known as paracetamol, is used as an analgesic and antipyretic in small doses, it has also significant antioxidant properties. In our work a few different configurations of cholesterol against acetaminophen were optimized by classical dynamics methods and then used as starting configurations for further DFT optimization. The binding energy, hydrogen bond formation, electron density and shapes of HOMO and LUMO molecular orbitals were calculated and analyzed. The calculated electronic properties of separated molecules and interacting molecules revealed substantial differences.

Figure 1. Electron density of interacting Acetaminophen and Cholesterol

1. *Weber C., Noels H.* Atherosclerosis: current pathogenesis and therapeutic options// Nature Medicine.-2011.-**17.-**P. 1410-1422.