

On the interaction of polyvinylpyrrolidone with carbon nanotubes to create a coating of medical stents.

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Technologies for creating thin-film coatings of medical stents with an extended time of drug emission for the treatment of various diseases have recently played an important role in modern medicine. A properly selected component that slows down the desorption of the drug can speed up the process of treating the disease. Carbon nanotubes (CNTs) added to the coating help to improve the physicochemical properties of the proposed component composition and increase the desorption time of the drug from the surface of the coated stent.

To determine the possibility of using carbon nanotubes as a component of the drug coating, we studied the mechanism of interaction of CNTs with the matrix component of the polyvinylpyrrolidone (PVP) coating. Quantum chemical calculations of the interaction of a PVP fragment containing 358 atoms and consisting of 21 monomers with a single-layer carbon nanotube (6, 6) using Density functional Theory have been performed. The atoms of the polyvinylpyrrolidone surface were chosen as the most likely adsorption centers during the interaction of the carrier polymer with the carbon nanotube: a carbon atom, an oxygen atom and a hydrogen atom. Modeling of the step-by-step approach of the CNT cluster to the selected center on the surface of the PVP is performed and energy curves of the processes are constructed.

The analysis of the obtained results showed that it is possible to create a stable complex consisting of PVP and CNT, and the complex is more energetically advantageous when the nanotube is attached to the hydrogen atom of the polyvinylpyrrolidone fragment (the interaction energy is -0.02 eV at a distance of 4 Å). When an oxygen atom, interaction is possible, but less advantageous from an energy point of view. In the case of CNT orientation to a carbon atom, the complex is unstable (the interaction energy is 2.18 eV at a distance of 3 Å).

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