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INTERACTION OF SERUM ALBUMIN AND GRAPHENE OXIDE: INVESTIGATION BY TRITIUM PROBE AND MOLECULAR DOCKING

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Graphene oxide (GO) modification with different compounds for synthesis of new materials with specified properties is the field of interest of modern investigation [1]. Since serum albumin is the main blood protein, it is important to understand the mechanisms of its interaction with medical materials. In present work we propose a novel complex approach of studying interactions between bovine serum albumin (BSA) and GO. The approach includes tritium probe method and computer simulation.
Tritium probe method is based on the application of tritium labeled compounds for the to determine the composition of composite materials, as well as to determine the structural organization of protein molecules on the surface of a solid substrate [2].
BSA was adsorbed on the solid of an aqueous suspension of GO. The composition of such prepared material was determined with the help of tritium labeled protein. We observed that BSA strongly adsorbs on GO. To reveal the structural peculiarities of protein on GO surface, the adsorption composite was subjected to bombardment with atomic tritium following by analysis of label distribution in the amino acid residues. Tritium atoms were formed from molecular tritium on the tungsten filament heated by the electric current up to 1830 K.
The experimental results were compared with molecular docking simulation. Molecular docking was performed using AutoDock Vina 1.2.3, LeDock and Hex8.0.0 softwires. Preliminary preparation of the carbon substrate model, minimization of the free energy of GO structure, as well as preparation of protein files for calculation were carried out using ChemBioDraw/3D Ultra 11.0.2., UCSF Chimera 1.15 respectively. The molecular modeling was performed tooking into account the presence of structural defects in GO, the hydrate shell on the surface of the nanocarbon substrate, as well as the formation of a "protein corona" due to protein-protein interactions.
As a result, we determined the composition of BSA-GO adsorption composites in the wide range of protein concentrations. Moreover, binding sites of BSA and GO have been identified, and the important role of histidine in protein retention on the GO surface will be discussed in the presentation.

1. Gusarova E.A. et al., Colloid and Interface Science Communications. 46, 100575 (2022).
2. Chernysheva M.G. et al., Radiochemistry. 63(2), 227 (2021).

The speaker is a student or young scientist

Yes

Section

1. Applications of nuclear methods in science and technology

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