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DFT computational studies of cellulose molecules adsorption on carbon nanostructures

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Cellulose is one of the most common biopolymers. It has high strength, flexible, and has the transparency in the optical range. Also, cellulose is very ecology and refers to renewable resources. Carbons nanostructure is low-size structures that carbon in the basic. They can be used to create high-strength conductive wires or to create nano sorbents that filter water and air. They are also used to create a thin and transparent conductive surface.

The work presents results of the computational studies of cellulose molecules adsorption on the surfaces of carbon nanostructures as part of the ab-initio method. Geometry-optimized calculations of the electronic structure of carbon nanostructures (graphene sheets and fragments of nanotubes) with adsorbed molecules (clusters) based on DFT were performed using the Gaussian 09 software package [1].

Relaxed geometries, binding energies, cellulose molecules in adsorbed and free states were calculated and analyzed, in this work. The results of the calculation were used for comparison with experimental data. Obtained results are discussed in view of potential use of cellulose-carbon composite materials in various optical and optoelectronic applications.

Topics

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