

Sensor Activity Of Carbon Nanotubes

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Abstract

High sensitivity of electronic characteristics of carbon nanotubes to existence on their border of adsorbed molecules or radicals [1, 2] speaks about creation possibility on this basis of the high-sensitivity super tiny sensor. With its help it will be possible to find availability of the slightest impurity in samples.

We studied the carbon nanotube which border was modified by carboxyl functional group - COOH (fig. 1). This system represents a test probe, capable to react to various chemical elements. For the proof of its sensor activity the theoretical researches of possible interaction of the modified single-walled arm-chair carbon nanotube type (6, 6) with atoms of alkaline metals were executed.

The quantum-chemical MNDO method within a molecular cluster was used. The process of accession of carboxyl group to the open border of nanotube was simulated and studied. Process of scanning by the test probe of any surface containing subject initialization atoms created thus is investigated, and activity of nanotube with the functional group to potassium, sodium, lithium and magnesium atoms is defined.

Process was modeled by step-by-step approach of metal atoms to hydrogen atom of functional group along the straight line parallel to modified border of the (6, 6) nanotube (fig. 1). Power curves of this process were constructed. The analysis of the constructed power curves found the fact of interaction between the modified nanotube and the chosen atoms (K, Na, Li, Mg). It is illustrated by characteristic minima on curves.

The received results proved possibility of use of the modified carbon nanotube as a sensor on certain elements and radicals.

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