Quantum-chemical modeling of electron-mechanical properties of nanotubes

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The work is devoted to the modernization of algorithms and the development of a software package for calculating and predicting the electronic and mechanical properties of a wide class of nanotubes from noble and non-ferrous metals.

The relevance of the work.

Nanotubes are very important new nanomaterials, the characteristics of which vary within certain limits. Miniature dimensions, unique physico-chemical and electronic properties motivate the development of these studies, contributing to an increase in the interest of engineers and researchers to nanotubes.

The most priority areas of nanotechnology are: the study of the structure and properties of nanotubes, the development of methods for their synthesis, as well as the expansion of their applications. A variety of electronic devices are created on the basis of nanotubes, up to the implementation of a computer, whose operation is based on the use of transistors exclusively on carbon nanotubes. Nanotubes can be subjected to mechanical deformation: twisting, stretching and compression along the axis, bending, flattening. At the same time, the physical properties of nanotubes and the operation of electronic elements based on them can be controlled by mechanical influences by changing the shape of nanotubes. The rapid development of this experimental field, called nanoelectromechanics, is limited by the lack of theoretical studies of the electromechanical properties of tubes.

To date, a variety of non-carbon nanotubes have been synthesized, up to tubes made of precious metals and compounds of transition elements. Theoretical modeling of the electronic and especially electromechanical properties of these nanomaterials is becoming an extremely urgent task.

The aim of the work. Based on the method of linearized coupled cylindrical waves, to modernize algorithms and develop a software package for calculating and predicting the electronic and mechanical properties of a wide class of nanotubes made of precious and non-ferrous metals.

The tasks of the work. To achieve the goal, the following tasks are set:

• Improve algorithms for calculating magnetic and electromagnetic fields in chiral nanotubes and create a software package for calculating the properties of nanotubes;

• To study ways to accelerate quantum-chemical modeling and optimize the computational process;

• Perform quantum-mechanical calculations of magnetic and electromagnetic fields in chiral nanotubes made of precious and non-ferrous metals;

• To study the effect of spin-orbit interaction on the electronic properties of nanotubes made of non-ferrous and precious metals;

• To study the effect of mechanical deformations on the electronic structure of precious metal tubes;

• To study electron and spin transport in chiral nanotubes made of precious metals.

Scientific novelty.

• Development of the theory of quantum-chemical calculations of the electronic properties of nanotubes of any composition by the method of linearized coupled cylindrical waves;

• It has been established that for gold, silver and copper nanotubes, the number of ballistic transport channels is equal to the sum of the chirality indices of the nanotubes;

• It has been established that the spin-orbit interaction manifests itself in the form of splitting of non-relativistic dispersion curves, which decreases during the transition to the internal states of the valence band and nanotubes of a larger radius;

• It has been established that with the help of mechanical deformations of tubes, it is possible to control the electronic properties of platinum and palladium tubes by adjusting the band gap in palladium tubes and the spin density of states in platinum nanotubes;

• It has been established that very large fields can be realized in nanoscale volumes using nanosolenoids made of chiral nanotubes.

• It is established that the frequencies of low-energy natural oscillations of the electromagnetic field depend on the radius of the nanotubes and lie in the X-ray range.

Theoretical and practical significance. A software package consisting of software modules has been developed that allows quantum-chemical modeling of the electron-mechanical properties of nanotubes, taking into account the spin-orbit interaction. The

obtained results of calculations of the properties of nanotubes can be used in the development of new ways of their application: gold, silver and copper nanotubes can be used in nanoelectronics as nanolenoids and radiating antennas; palladium and platinum nanotubes – in spintronics as sensors.

Statements submitted for defense:

1. Methods for calculating magnetic and electromagnetic fields in chiral nanotubes;
2. Block diagram of algorithms for creating software modules for calculating electromagnetic fields in chiral nanotubes;
3. The results of modeling the electronic band structure taking into account the spin-orbit interaction of nanotubes of various types of precious and non-ferrous metals;
4. Results of modeling the electronic properties of nanotubes with internal nanowires made of transition metals;
5. Results of modeling the effect of mechanical deformations on the electronic structure of nanotubes made of precious metals;
6. Results of modeling magnetic and electromagnetic fields in chiral nanotubes made of precious metals.