The quantum chemical research of the dependence of SWCN's dipole moment

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It is interesting to investigate the possibility of using carbon nanotubes [1] as some electronic gauges. The main feature of carbon nanotube which can be used in the gauges is dipole moment. We have considered the fragments of single-wall polarized carbon nanotubes (n, n) and (n, 0) types (n = 3, 4). The unsaturated cluster boundary chemical bonds have been completed by some atoms (or groups of atoms) on the both sides. The length of tubes has been varied. The electronic structure and energetic properties of nanotubes were calculated by applying the semi-empirical methods of quantum chemistry [2].

The results of the calculation have shown that the dependence of the dipole moment from the length of nanotubes has a nonlinear character and dipole moment value is depending on the boundary atom types. The values of the dipole moment of carbon nanotubes oscillate and these oscillations are different for each of the tube's types. But the oscillations are less pronounced with increasing the diameter of (n, n) type of nanotubes and the curves become smoother. For (n, 0) type of nanotubes such dependence is not observed.

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[1] Harris P. Carbon nanotubes and related structures. New materials of the XXI century. - M: the Technosphere, 2003.
[2] Stepanov N.F. Quantum mechanics and quantum chemistry. - M: Mir, 2001.