ТЕЗИСЫ ДОКЛАДОВ

INTERNATIONAL WORKSHOP

«Multiscale Biomechanics and Tribology of Inorganic and Organic Systems»

МЕЖДУНАРОДНАЯ КОНФЕРЕНЦИЯ

«Перспективные материалы с иерархической структурой для новых технологий и надежных конструкций»

VIII ВСЕРОССИЙСКАЯ НАУЧНО-ПРАКТИЧЕСКАЯ КОНФЕРЕНЦИЯ С МЕЖДУНАРОДНЫМ УЧАСТИЕМ, ПОСВЯЩЕННАЯ 50-ЛЕТИЮ ОСНОВАНИЯ ИНСТИТУТА ХИМИИ НЕФТИ

«Добыча, подготовка, транспорт нефти и газа»

Томск
Издательский Дом ТГУ
2019

DOI: 10.17223/9785946218412/111

COMPUTER SIMULATION OF QUANTUM TECHNOLOGIES: A_2 (A = C, Si, N, P, O, S) DIMMER SENSORS BASED ON SINGLE-WALL CARBON NANOTUBES

[1]Maslova O.A., [1]Beznosyuk S.A., [2]Masalimov A.S.
[1]Altai state university, Barnaul
[2]Karaganda state university, Karaganda

The accelerating second quantum revolution of technologies assumes the use of specific non-local quantum entangled systems of subatomic attosecond and supraatomic femtosecond scale levels of materials [1]. The use of single-wall carbon nanotubes (SWCNTs) is now considered to develop highly sensitive femtosecond specific quantum sensors at supraatomic nanosized scale [2]. Today it is known that SWCNTs are very sensitive to molecules such as NH_3, NO_2, C_2H_4, CO, SO_2, H_2S, H_2, N_2, O_2, [3, 4].

In this regard, the theoretical study of the femtochemistry quantum processes different atoms on nano-sized surfaces of SWCNTs is very relevant. It is carried out within the framework of this work using quantum chemical methods of computer simulation. The purpose of this work is to study the adsorption of diatomic A_2 molecules (A = C, Si, N, P, O, S) by a SWCNT having a minimum length and diameter. The choice of molecules is determined by the need to compare the adsorption characteristics of dimers belonging to group IV (C, Si), group V (N, P) and group VI (O, S) of the second and third periods of the table of chemical elements. This paper presents the theoretical study of quantum-chemical solution of one of the most urgent tasks in the development of a new generation of supra-atomic femtosecond sensors of molecules on the basis of SWCNTs.

Fig. 1 shows the attack by the diatomic A_2 molecule of the sensor outer surface (left). Here h is the distance from the SWCNT outer surface to the dimer atom nearest to it. On the Fig. 2 there are three points (T, B, C) of the diatomic A_2 molecule landing on the SWCNT outer surface.

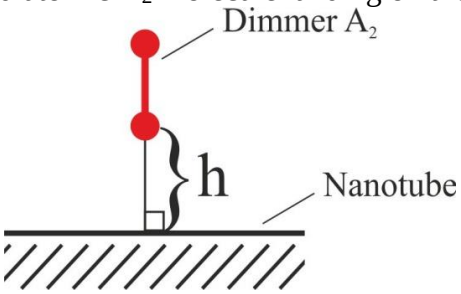

Fig 1. Model of the diatomic A_2 molecule adsorption on the SWCNT outer surface

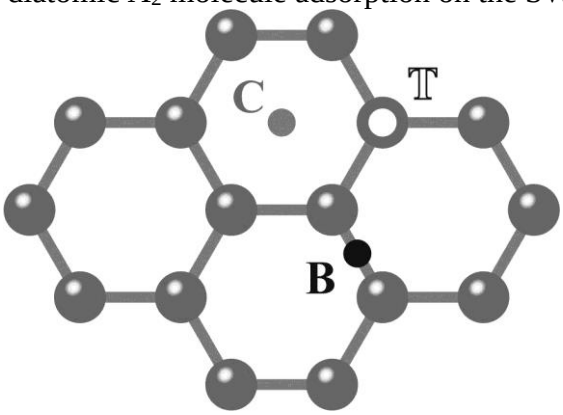

Fig 2. Three points (T, B, C) of the diatomic A_2 molecule landing on the SWCNT outer surface.

Numerical simulation is performed using the approach that was considered in a previous paper [5]. Modeling and calculations are performed in two stages. At the first stage, a study is made of the stable configuration of the SWCNT having the minimum diameter and the minimum length. At the second stage, simulations of attacks with different orientation of the A_2 (A = C, Si, N, P, O, S) molecules of different landing sites on outer surface of the sensors are performed. The Kohn-Shem method is used in the local density functional approximation LDA / 3-21G (ORCA package [6]) to model the potential energy surface (PES) of the sensor nanosystems.

A study of femtosecond sensors of the supra-atomic range of the nanoscale based on the SWNTs sensor has shown the possibility of an adequate description of such sensory nanosystems in a multilevel hierarchy of functional elements of intelligent materials using modern density functional methods.

From the obtained results it follows that the axes of all molecules are perpendicular to the outer surface of the sensor, as shown in Fig. 1. We considered three positions of landing of the molecules presented in fig. 2: above the carbon atom, above a pair of carbon atoms and the center of the sextet of carbon atoms. According to the results of calculations, we note significant differences in the adsorption characteristics of diatomic molecules of groups IV (C, Si), V (N, P) and VI (O, S) of the second and third periods. In case of C_2, Si_2 molecules, it is chemisorption. In turn, for the O_2, S_2, and N_2, P_2 molecules, it is a variant of physical adsorption. In a case of C_2 molecule, it is more preferable to adsorb on a pair of C-C atoms, and for the Si_2 molecule it is energetically advantageous to attach one carbon atom C. For molecules O_2, S_2, N_2, P_2 it is preferable to attach in the center of the carbon sextet C_6.

By analyzing the PES of quantum nanomolecular sensor systems, the following conclusions were obtained:

- The results of the quantum chemical calculations performed are in agreement with the published data of other authors for the SWCNT sensors in cases of molecules O_2 and N_2.
- Linking all investigated dimmers with an axial orientation perpendicular to the outer surface of the SWCNT sensor is an energetically beneficial exothermic process.
- The SWCNT sensor binds C_2, Si_2 molecules with energies of 2.91 eV and 1.51 eV, respectively. This is chemisorption.
- The most stable is the position of the C_2 molecule at an equilibrium distance of 1.39 Å from the outer surface of the SWCNT sensor between a pair of adjacent carbon atoms C - C, and in the case of Si_2 – at an equilibrium distance of 2.13 Å above the carbon atom in the SWCNT sensor.
- For the O_2, S_2, N_2, P_2 molecules, the energies of attachment to a single-walled CNT are: 0.39 eV, 0.52 eV, 0.15 eV, and 0.27 eV, respectively. This is an order of magnitude less than for the adsorption of C_2 and Si_2 molecules.
- The most stable arrangement of O_2, S_2, N_2, P_2 molecules occurs in the center of the carbon sextet C_6 of the SWCNT sensor at distances: 2.66 Å, 2.96 Å, 3.00 Å and 3.17 Å respectively. Low binding energies and positioning indicate a physical type of adsorption.

The data obtained may be useful in further studying the growth process and the formation of the infrastructure of femtosecond sensors at the supra-atomic level of carbon nanomaterials in order to change and improve their original properties, as well as in studying the adsorption of diatomic molecules by carbon nanotubes, in the development of gas sensors based on the SWCNT.

1.Beznosyuk S.A. and Zhukovsky M.S. Multiscale space-time dissipative structures in materials: two-electron genesis of nonequilibrium electromechanical interfaces // Phys. Mesomechanics. 2017.- Vol. 20(1). P. 102–110.
2. Steinhauser M.O. Computational Multiscale Modeling of Fluids and Solids: Theory and Applications, 2nd ed., Springer-Verlag, Berlin, Heidelberg. 2017. - 419 p.
3. Lan Y., Wang Y., Ren F. Physics and applications of aligned carbon nanotube // Advances in Physics. 2011 - №4. P. 553-678.
4. Fahimen S. N_2 adsorption on the inside and outside the single-walled carbon nanotubes by density functional theory study// J. Phys. 2018. - №4. P. 2–15.
5. Beznosyuk S.A., Maslova O.A., Zhukovsky M.S., et al. Mathematical modeling of the infrastructure of attosecond actuators and femtosecond sensors of nonequilibrium physical media in smart materials // AIP Conf. Proc. 2017. - №1909. P. 020014-1 – 020014-5.
6. Neese F The ORCA program system. Wiley interdisciplinary Reviews //Comput. Mol. Sci., 2012, Vol 2., Issue 1, P. 73–78.